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(54) ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

(57) A compound that has the structure according to Formula $M(L_A)_x(L_B)_y(L_C)_z$: wherein ligand L_A is



ligand L_B is



; and ligand L_C is



and devices and formulations containing these compounds are disclosed. In Formula $M(L_A)_x(L_B)_y(L_C)_z$: M is a metal having an atomic number greater than 40;

x is 1 or 2;

x+y+z is the oxidation state of the metal M;

X¹-X⁴ and A¹-A⁸ are C or N;

at least one of A^1 - A^8 is N;

X is O, S, or Se;

two adjacent R^B form a six-member aromatic ring E fused to ring B; wherein ring E can be substituted by R^E;

each R^A-R^E and R¹-R⁴ is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfanyl, sulfonyl, phosphino, and combinations thereof.



FIGURE 1

Description

PARTIES TO A JOINT RESEARCH AGREEMENT

5 [0001] The claimed invention was made by, on behalf of, and/or in connection with one or more of the following parties to a joint university corporation research agreement: Regents of the University of Michigan, Princeton University, University of Southern California, and the Universal Display Corporation. The agreement was in effect on and before the date the claimed invention was made, and the claimed invention was made as a result of activities undertaken within the scope of the agreement.

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FIELD OF THE INVENTION

[0002] The present invention relates to compounds for use as emitters and devices, such as organic light emitting diodes, including the same.

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BACKGROUND

[0003] Opto-electronic devices that make use of organic materials are becoming increasingly desirable for a number of reasons. Many of the materials used to make such devices are relatively inexpensive, so organic opto-electronic 20 devices have the potential for cost advantages over inorganic devices. In addition, the inherent properties of organic materials, such as their flexibility, may make them well suited for particular applications such as fabrication on a flexible substrate. Examples of organic opto-electronic devices include organic light emitting devices (OLEDs), organic phototransistors, organic photovoltaic cells, and organic photodetectors. For OLEDs, the organic materials may have performance advantages over conventional materials. For example, the wavelength at which an organic emissive layer

- 25 emits light may generally be readily tuned with appropriate dopants. [0004] OLEDs make use of thin organic films that emit light when voltage is applied across the device. OLEDs are becoming an increasingly interesting technology for use in applications such as flat panel displays, illumination, and backlighting. Several OLED materials and configurations are described in U.S. Pat. Nos. 5,844,363, 6,303,238, and 5,707,745, which are incorporated herein by reference in their entirety.
- 30 [0005] One application for phosphorescent emissive molecules is a full color display. Industry standards for such a display call for pixels adapted to emit particular colors, referred to as "saturated" colors. In particular, these standards call for saturated red, green, and blue pixels. Color may be measured using CIE coordinates, which are well known to the art.

[0006] One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted Ir(ppy)₃, which has the following structure:

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- [0007] In this, and later figures herein, we depict the dative bond from nitrogen to metal (here, Ir) as a straight line. 45 [0008] As used herein, the term "organic" includes polymeric materials as well as small molecule organic materials that may be used to fabricate organic opto-electronic devices. "Small molecule" refers to any organic material that is not a polymer, and "small molecules" may actually be quite large. Small molecules may include repeat units in some circumstances. For example, using a long chain alkyl group as a substituent does not remove a molecule from the "small
- 50 molecule" class. Small molecules may also be incorporated into polymers, for example as a pendent group on a polymer backbone or as a part of the backbone. Small molecules may also serve as the core molety of a dendrimer, which consists of a series of chemical shells built on the core moiety. The core moiety of a dendrimer may be a fluorescent or phosphorescent small molecule emitter. A dendrimer may be a "small molecule," and it is believed that all dendrimers currently used in the field of OLEDs are small molecules.
- 55 [0009] As used herein, "top" means furthest away from the substrate, while "bottom" means closest to the substrate. Where a first layer is described as "disposed over" a second layer, the first layer is disposed further away from substrate. There may be other layers between the first and second layer, unless it is specified that the first layer is "in contact with" the second layer. For example, a cathode may be described as "disposed over" an anode, even though there are various

organic layers in between.

[0010] As used herein, "solution processible" means capable of being dissolved, dispersed, or transported in and/or deposited from a liquid medium, either in solution or suspension form.

[0011] A ligand may be referred to as "photoactive" when it is believed that the ligand directly contributes to the photoactive properties of an emissive material. A ligand may be referred to as "ancillary" when it is believed that the ligand does not contribute to the photoactive properties of an emissive material, although an ancillary ligand may alter the properties of a photoactive ligand.

[0012] As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher

- 10 than" a second HOMO or LUMO energy level if the first energy level is closer to the vacuum energy level. Since ionization potentials (IP) are measured as a negative energy relative to a vacuum level, a higher HOMO energy level corresponds to an IP having a smaller absolute value (an IP that is less negative). Similarly, a higher LUMO energy level corresponds to an electron affinity (EA) having a smaller absolute value (an EA that is less negative). On a conventional energy level diagram, with the vacuum level at the top, the LUMO energy level of a material is higher than the HOMO energy level
- ¹⁵ of the same material. A "higher" HOMO or LUMO energy level appears closer to the top of such a diagram than a "lower" HOMO or LUMO energy level.

[0013] As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum level, this means that a "higher" work function is more

20 negative. On a conventional energy level diagram, with the vacuum level at the top, a "higher" work function is illustrated as further away from the vacuum level in the downward direction. Thus, the definitions of HOMO and LUMO energy levels follow a different convention than work functions.

[0014] More details on OLEDs, and the definitions described above, can be found in US Pat. No. 7,279,704, which is incorporated herein by reference in its entirety.

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SUMMARY OF THE INVENTION

[0015] According to an embodiment, a compound is provided that has the structure of Formula $M(L_A)_x(L_B)_y(Lc)_z$: wherein ligand L_A is

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ligand L_B is



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;

and ligand ${\rm L}_{\rm C}$ is



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[0016] In the compound of Formula $M(L_A)_x(L_B)_y(Lc)_z$:

	M is a metal having an atomic number greater than 40;
15	x is 1, or 2;
	y is 0, 1, or 2;
	z is 0, 1, or 2;
	x+y+z is the oxidation state of the metal M;
	X ¹ , X ² , X ³ , X ⁴ , A ¹ , A ² , A ³ , A ⁴ , A ⁵ , A ⁶ , A ⁷ , and A ⁸ are C or N;
20	at least one of A ¹ , A ² , A ³ , A ⁴ , A ⁵ , A ⁶ , A ⁷ , and A ⁸ is N;
	ring B is bonded to ring A through a C-C bond;
	M is bonded to ring A through a M-C bond;
	X is O, S, or Se;
	rings C, and D are each independently a 5 or 6-membered carbocyclic or heterocyclic ring;
25	R ^A represents mono, or di-substitution, or no substitution;
	R ^B represents di, tri, or tetra-substitution;
	R ^C , R ^D , and R ⁴ each independently represent mono, di, tri, or tetra-substitution, or no substitution;
	two adjacent R ^B form a six-member aromatic carbocyclic or heterocyclic ring E fused to ring B; wherein, when ring
	E is heterocyclic, the only heteroatom is nitrogen; wherein ring E can be further substituted by R ^E ; and wherein R ^E
30	represents mono, di, tri, or tetra-substitution, or no substitution;
	each of R ^A , R ^B , R ^C , R ^D , R ^E , R ¹ , R ² , R ³ , and R ⁴ are independently selected from the group consisting of hydrogen,
	deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heter-
	oalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl,
	phosphino, and combinations thereof: and

³⁵ any adjacent substitutents of R^C, and R^D are optionally joined to form a fused ring.

[0017] According to another embodiment, a first device comprising a first organic light emitting device is also provided. The first organic light emitting device can include an anode, a cathode, and an organic layer, disposed between the anode and the cathode. The organic layer can include a compound of Formula $M(L_A)_x(L_B)_y(L_c)_z$. The first device can be a consumer product, an organic light-emitting device, and/or a lighting panel.

[0018] According to another embodiment, a formulation that includes a compound of Formula $M(L_A)_x(L_B)_y(Lc)_z$ is also provised.

BRIEF DESCRIPTION OF THE DRAWINGS

[0019]

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FIG. 1 shows an organic light emitting device.

⁵⁰ FIG. 2 shows an inverted organic light emitting device that does not have a separate electron transport layer.

FIG. 3 shows ligands $L_{\text{A}},\,L_{\text{B}},\,\text{and}\,\,L_{\text{C}}$ as disclosed herein.

DETAILED DESCRIPTION

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[0020] Generally, an OLED comprises at least one organic layer disposed between and electrically connected to an anode and a cathode. When a current is applied, the anode injects holes and the cathode injects electrons into the organic layer(s). The injected holes and electrons each migrate toward the oppositely charged electrode. When an

electron and hole localize on the same molecule, an "exciton," which is a localized electron-hole pair having an excited energy state, is formed. Light is emitted when the exciton relaxes via a photoemissive mechanism. In some cases, the exciton may be localized on an excimer or an exciplex. Non-radiative mechanisms, such as thermal relaxation, may also occur, but are generally considered undesirable.

⁵ **[0021]** The initial OLEDs used emissive molecules that emitted light from their singlet states ("fluorescence") as disclosed, for example, in U.S. Pat. No. 4,769,292, which is incorporated by reference in its entirety. Fluorescent emission generally occurs in a time frame of less than 10 nanoseconds.

[0022] More recently, OLEDs having emissive materials that emit light from triplet states ("phosphorescence") have been demonstrated. Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices,"

- Nature, vol. 395, 151-154, 1998; ("Baldo-I") and Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," Appl. Phys. Lett., vol. 75, No. 3, 4-6 (1999) ("Baldo-II"), which are incorporated by reference in their entireties. Phosphorescence is described in more detail in US Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.
- [0023] FIG. 1 shows an organic light emitting device 100. The figures are not necessarily drawn to scale. Device 100 may include a substrate 110, an anode 115, a hole injection layer 120, a hole transport layer 125, an electron blocking layer 130, an emissive layer 135, a hole blocking layer 140, an electron transport layer 145, an electron injection layer 150, a protective layer 155, a cathode 160, and a barrier layer 170. Cathode 160 is a compound cathode having a first conductive layer 162 and a second conductive layer 164. Device 100 may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in US 7 279 704 at cols. 6-10, which are incorporated by reference.
- in US 7,279,704 at cols. 6-10, which are incorporated by reference.
 [0024] More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F₄-TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and
- ²⁵ host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electrically-
- 30 conductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.
- ³⁵ [0025] FIG. 2 shows an inverted OLED 200. The device includes a substrate 210, a cathode 215, an emissive layer 220, a hole transport layer 225, and an anode 230. Device 200 may be fabricated by depositing the layers described, in order. Because the most common OLED configuration has a cathode disposed over the anode, and device 200 has cathode 215 disposed under anode 230, device 200 may be referred to as an "inverted" OLED. Materials similar to those described with respect to device 100 may be used in the corresponding layers of device 200. FIG. 2 provides one example of how some layers may be omitted from the structure of device 100.
- **[0026]** The simple layered structure illustrated in FIGS. 1 and 2 is provided by way of nonlimiting example, and it is understood that embodiments of the invention may be used in connection with a wide variety of other structures. The specific materials and structures described are exemplary in nature, and other materials and structures may be used. Functional OLEDs may be achieved by combining the various layers described in different ways, or layers may be
- ⁴⁵ omitted entirely, based on design, performance, and cost factors. Other layers not specifically described may also be included. Materials other than those specifically described may be used. Although many of the examples provided herein describe various layers as comprising a single material, it is understood that combinations of materials, such as a mixture of host and dopant, or more generally a mixture, may be used. Also, the layers may have various sublayers. The names given to the various layers herein are not intended to be strictly limiting. For example, in device 200, hole transport layer
- ⁵⁰ 225 transports holes and injects holes into emissive layer 220, and may be described as a hole transport layer or a hole injection layer. In one embodiment, an OLED may be described as having an "organic layer" disposed between a cathode and an anode. This organic layer may comprise a single layer, or may further comprise multiple layers of different organic materials as described, for example, with respect to FIGS. 1 and 2.
- [0027] Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247,190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. 1 and 2. For example, the substrate

may include an angled reflective surface to improve out-coupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

[0028] Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable

- 5 method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. Pat. No. 7,431,968, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes.
- 10 Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink-jet and OVJD. Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For
- 15 example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution processibility than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo 20
- solution processing.

[0029] Devices fabricated in accordance with embodiments of the present invention may further optionally comprise a barrier layer. One purpose of the barrier layer is to protect the electrodes and organic layers from damaging exposure to harmful species in the environment including moisture, vapor and/or gases, etc. The barrier layer may be deposited over, under or next to a substrate, an electrode, or over any other parts of a device including an edge. The barrier layer

- 25 may comprise a single layer, or multiple layers. The barrier layer may be formed by various known chemical vapor deposition techniques and may include compositions having a single phase as well as compositions having multiple phases. Any suitable material or combination of materials may be used for the barrier layer. The barrier layer may incorporate an inorganic or an organic compound or both. The preferred barrier layer comprises a mixture of a polymeric material and a non-polymeric material as described in U.S. Pat. No. 7,968,146, PCT Pat. Application Nos.
- 30 PCT/US2007/023098 and PCT/US2009/042829, which are herein incorporated by reference in their entireties. To be considered a "mixture", the aforesaid polymeric and non-polymeric materials comprising the barrier layer should be deposited under the same reaction conditions and/or at the same time. The weight ratio of polymeric to non-polymeric material may be in the range of 95:5 to 5:95. The polymeric material and the non-polymeric material may be created from the same precursor material. In one example, the mixture of a polymeric material and a non-polymeric material 35 consists essentially of polymeric silicon and inorganic silicon.
- [0030] Devices fabricated in accordance with embodiments of the invention may be incorporated into a wide variety of consumer products, including flat panel displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, heads up displays, fully transparent displays, flexible displays, laser printers, telephones, cell phones, personal digital assistants (PDAs), laptop computers, digital cameras, camcorders,
- 40 viewfinders, micro-displays, 3-D displays, vehicles, a large area wall, theater or stadium screen, or a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present invention, including passive matrix and active matrix. Many of the devices are intended for use in a temperature range comfortable to humans, such as 18 degrees C. to 30 degrees C., and more preferably at room temperature (20-25 degrees C), but could be used outside this temperature range, for example, from -40 degree C to + 80 degree C.
- 45 [0031] The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may employ the materials and structures. [0032] The term "halo" or "halogen" as used herein includes fluorine, chlorine, bromine, and iodine.
- [0033] The term "alkyl" as used herein contemplates both straight and branched chain alkyl radicals. Preferred alkyl 50 groups are those containing from one to fifteen carbon atoms and includes methyl, ethyl, propyl, isopropyl, butyl, isobutyl, tert-butyl, and the like. Additionally, the alkyl group may be optionally substituted.

[0034] The term "cycloalkyl" as used herein contemplates cyclic alkyl radicals. Preferred cycloalkyl groups are those containing 3 to 7 carbon atoms and includes cyclopropyl, cyclopentyl, cyclohexyl, and the like. Additionally, the cycloalkyl group may be optionally substituted.

55 [0035] The term "alkenyl" as used herein contemplates both straight and branched chain alkene radicals. Preferred alkenyl groups are those containing two to fifteen carbon atoms. Additionally, the alkenyl group may be optionally substituted.

[0036] The term "alkynyl" as used herein contemplates both straight and branched chain alkyne radicals. Preferred

alkyl groups are those containing two to fifteen carbon atoms. Additionally, the alkynyl group may be optionally substituted. [0037] The terms "aralkyl" or "arylalkyl" as used herein are used interchangeably and contemplate an alkyl group that has as a substituent an aromatic group. Additionally, the aralkyl group may be optionally substituted.

- [0038] The term "heterocyclic group" as used herein contemplates aromatic and non-aromatic cyclic radicals. Heteroaromatic cyclic radicals also means heteroaryl. Preferred hetero-non-aromatic cyclic groups are those containing 3 or 7 ring atoms which includes at least one hetero atom, and includes cyclic amines such as morpholino, piperdino, pyrrolidino, and the like, and cyclic ethers, such as tetrahydrofuran, tetrahydropyran, and the like. Additionally, the heterocyclic group may be optionally substituted.
- [0039] The term "aryl" or "aromatic group" as used herein contemplates single-ring groups and polycyclic ring systems. The polycyclic rings may have two or more rings in which two carbons are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is aromatic, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Additionally, the aryl group may be optionally substituted, and may comprise, e.g., six to twenty carbon atoms.
- [0040] The term "heteroaryl" as used herein contemplates single-ring hetero-aromatic groups that may include from one to three heteroatoms and three to twenty carbon atoms, for example, pyrrole, furan, thiophene, imidazole, oxazole, thiazole, triazole, pyrazole, pyridine, pyrazine and pyrimidine, and the like. The term heteroaryl also includes polycyclic hetero-aromatic systems having two or more rings in which two atoms are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is a heteroaryl, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Additionally, the heteroaryl group may be optionally substituted.
- ²⁰ **[0041]** The alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, heterocyclic group, aryl, and heteroaryl may be optionally substituted with one or more substituents selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, cyclic amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.
- ²⁵ **[0042]** As used herein, "substituted" indicates that a substituent other than H is bonded to the relevant position, such as carbon. Thus, for example, where R¹ is mono-substituted, then one R¹ must be other than H. Similarly, where R¹ is di-substituted, then two of R¹ must be other than H. Similarly, where R¹ is unsubstituted, R¹ is hydrogen for all available positions.
- **[0043]** The "aza" designation in the fragments described herein, i.e. aza-dibenzofuran, azadibenzonethiophene, etc. means that one or more of the C-H groups in the respective fragment can be replaced by a nitrogen atom, for example, and without any limitation, azatriphenylene encompasses both dibenzo[*f*,*h*]quinoxaline and dibenzo[*f*,*h*]quinoline. One of ordinary skill in the art can readily envision other nitrogen analogs of the aza-derivatives described above, and all such analogs are intended to be encompassed by the terms as set forth herein.
- [0044] It is to be understood that when a molecular fragment is described as being a substituent or otherwise attached to another moiety, its name may be written as if it were a fragment (e.g. naphthyl, dibenzofuryl) or as if it were the whole molecule (e.g. naphthalene, dibenzofuran). As used herein, these different ways of designating a substituent or attached fragment are considered to be equivalent.

[0045] The novel ligands disclosed herein can be used to produce metal complexes that are useful in emissive devices. The incorporation of these ligands allows red phosphorescent materials with good external quantum efficiency (EQE), good color, and good lifetime.

[0046] According to one embodiment, a compound is disclosed that has a structure according to Formula $M(L_A)_x(L_B)_v(Lc)_z$: wherein ligand L_A is

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ligand L_B is

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¹⁰ and ligand L_C is

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[0047] In the compound of Formula $M(L_A)_x(L_B)_y(Lc)_z$:

ethyl, and combinations thereof.

25	M is a metal having an atomic number greater than 40; x is 1, or 2; y is 0, 1, or 2;
	z is 0, 1, or 2;
	x+y+z is the oxidation state of the metal M;
30	X ¹ , X ² , X ³ , X ⁴ , A ¹ , A ² , A ³ , A ⁴ , A ⁵ , A ⁶ , A ⁷ , and A ⁸ are C or N;
	at least one of A ¹ , A ² , A ³ , A ⁴ , A ⁵ , A ⁶ , A ⁷ , and A ⁸ is N;
	ring B is bonded to ring A through a C-C bond;
	M is bonded to ring A through a M-C bond;
	X is O, S, or Se;
35	rings C, and D are each independently a 5 or 6-membered carbocyclic or heterocyclic ring;
	R ^A represents mono, or di-substitution, or no substitution;
	R ^B represents di, tri, or tetra-substitution;
	R ^C , R ^D , and R ⁴ each independently represent mono, di, tri, or tetra-substitution, or no substitution;
	two adjacent R ^B form a six-member aromatic carbocyclic or heterocyclic ring E fused to ring B; wherein, when ring
40	E is heterocyclic, the only heteroatom is nitrogen; wherein ring E can be further substituted by R ^E ; and wherein R ^E
	represents mono, di, tri, or tetra-substitution, or no substitution;
	each of R ^A , R ^B , R ^C , R ^D , R ^E , R ¹ , R ² , R ³ , and R ⁴ are independently selected from the group consisting of hydrogen,
	deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heter-
	oalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl,
45	phosphino, and combinations thereof; and

any adjacent substitutents of R^C, and R^D are optionally joined to form a fused ring.

[0048] In some embodiments, none of the adjacent R^E substituents are fused *(i.e., all R^E are unfused)*. In some embodiments, each R^E is independently selected from the group consisting of hydrogen, deuterium, alkyl, cycloalkyl, aryl, while each R^E is independently selected from the group consisting of hydrogen or alkyl in other embodiments. In some embodiments, at least one R^E has at least two carbons, while at least one R^E has at least three carbons or at least four carbons in other embodiments. In some embodiments, each R⁴ is independently selected from the group consisting of H, D, alkyl, and com-

binations thereof. In some embodiments, each R⁴ is independently selected from the group consisting of H, D, methyl, ethyl, isopropyl, propyl, butyl, isobutyl, and combinations thereof.
[0050] In some embodiments, each R^A is independently selected from the group consisting of H, D, alkyl, and combinations thereof. In some embodiments, each R^A is independently selected from the group consisting of H, D, methyl, binations thereof. In some embodiments, each R^A is independently selected from the group consisting of H, D, methyl, binations thereof.

[0051] In some embodiments, M is selected from the group consisting of Ir, Rh, Re, Ru, Os, Pt, Au, and Cu. In some embodiments, M is Ir. In some embodiments, X is O.

[0052] In some embodiments, the compound has the formula $M(L_A)_2(L_B)$. In other embodiments, the compound has the formula $M(L_A)(L_C)_2$.

[0053] In some embodiments, only one of A¹ to A⁸ is N. In some embodiments, only one of A⁵ to A⁸ is N. In some embodiments, X¹, X², X³, and X⁴ are C, and ring E is benzene. In other embodiments, (a) at least one of X¹, X², X³, and X⁴ is N, (b) ring E is heterocylic, or (c) both. In some embodiments, ring C is benzene and ring D is pyridine.
 [0054] In some embodiments, L_A has the formula:





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[0055] In some more specific embodiments, wherein L_A has the formula:



⁴⁰ wherein R is selected from the group consisting of alkyl, cycloalkyl, and combinations thereof. In some embodiments, R is selected from the group consisting of methyl, ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, cyclopentyl, cyclohexyl, partially or fully deuterated variants thereof, and combinations thereof. [0056] In some embodiments, L_B has the formula:

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⁵⁵ wherein R⁵, R⁶, R⁷, and R⁸ are independently selected from group consisting of alkyl, cycloalkyl, aryl, and heteroaryl; and wherein at least one of R⁵, R⁶, R⁷, and R⁸ has at least two C atoms.

[0057] In some embodiments, each R¹, R², R³, R^C, and R^D is independenly selected from group consisting of hydrogen, deuterium, alkyl, cycloalkyl, and combinations thereof. In some embodiments, R³ is hydrogen. In some embodiments,

each R¹, R², R³, R^C, and R^D is independently selected from the group consisting of methyl, ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, 2-methylpropyl, 2-methylpropyl, 1.2-dimethylpropyl, 2.2-dimethylpropyl, cyclobutyl, cyclopentyl, cyclohexyl, partially or fully deuterated variants thereof, and combinations thereof.

⁵ [0058] In some more specific embodiments, the compound is selected from the group consisting of:



and

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wherein each of R^F, R^G, R^H, R^I, R^J, and R^K are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and wherein X⁵, X⁶, X⁷, and X⁸ are C or N.

[0059] In some specific embodiments, L_A is selected from the group consisting of:

 L_{A1} through L_{A13} , each represented by the formula





LA14 through LA26, each represented by the formula



wherein in L_{A14} , R = H, and R^A = H, in L_{A15} , R = H, and R^A = CH₃, in L_{A16} , R = H, and R^A = CD₃, in L_{A17} , R = CH₃, and R^A = H, in L_{A18} , R = CD₃, and R^A = H, in L_{A19} , R = CH₃, and R^A = CH₃, in L_{A20} , R = CD₃, and R^A = CD₃, in L_{A21} , R = Ethyl, and R^A = H, in L_{A22} , R = Ethyl, and R^A = CH₃, in L_{A23} , R = Ethyl-*d5*, and R^A = CD₃, in L_{A24} , R = isopropyl, and R^A = H, (continued)

in L_{A12} , R = isopropyl, and R^A = CH₃, in L_{A13} , R = isopropyl-*d*7, and R^A = CD₃,

 L_{A27} through L_{A39} , each represented by the formula



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	wherein in L _{A27} , R = H, and R ^A = H,
15	in L_{A28} : R = H, and R ^A = CH ₃ ,
	in L_{A29} : R = H, and R ^A = CD ₃ ,
	in L_{A30} : R = CH ₃ , and R ^A = H,
	in L _{A31} : R = CD ₃ , and R ^A = H,
	in L_{A32} : R = CH ₃ , and R ^A = CH ₃ ,
20	in L_{A33} : R = CD ₃ , and R ^A = CD ₃ ,
	in L_{A34} : R = Ethyl, and R ^A = H,
	in L_{A35} R = Ethyl, and $R^A = CH_3$,
	in L_{A36} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
25	in L _{A37} : R = isopropyl, and R ^A = H,
	in L_{A38} : R = isopropyl, and R ^A = CH ₃ ,
	in L_{A39} : R = isopropyl-d7, and R ^A = CD ₃ ,

 L_{A53} through $L_{A65},$ each represented by the formula

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35	R-C-RA
	wherein in L_{A53} : R = H, and R ^A = H,

	in L_{A54} : R = H, and R ^A = CH ₃ ,
40	in L_{A55} R = H, and R ^A = CD ₃ ,
40	in L_{A56} : R = CH ₃ , and R ^A = H,
	in L_{A57} : R = CD ₃ , and R ^A = H,
	in L_{A58} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A59} : R = CD ₃ , and R ^A = CD ₃ ,
45	in L_{A60} : R = Ethyl, and R ^A = H,
	in L_{A61} : R = Ethyl, and R ^A = CH ₃ ,
	in L_{A62} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
	in L_{A63} : R = isopropyl, and R ^A = H,
50	in L_{A64} : R = isopropyl, and R ^A = CH ₃ ,
50	in L_{A65} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ ,

 L_{A79} through L_{A91} , each represented by the formula

in L_{A25}, R = isopropyl, and R^A = CH₃, in L_{A26}, R = isopropyl-*d*7, and R^A = CD3, L_{A40} through L_{A52}, each represented by the formula



wherein in L_{A40} : R = H, and R^A = H, in L_{A41} : R = H, and R^A = CH₃, in L_{A42} : R = H, and R^A = CD₃, in L_{A43} : R = CH₃, and R^A = H, in L_{A44} : R = CD₃, and R^A = H, in L_{A45} : R = CH₃, and R^A = CH₃, in L_{A46} : R = CD₃, and R^A = CH₃, in L_{A46} : R = CD₃, and R^A = CH₃, in L_{A47} : R = Ethyl, and R^A = H, in L_{A48} : R = Ethyl, and R^A = CH₃, in L_{A49} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A50} : R = isopropyl, and R^A = CH₃, in L_{A51} : R = isopropyl, and R^A = CH₃, in L_{A52} : R = isopropyl-*d7*, and R^A = CD₃,

 L_{A66} through $L_{A78},$ each represented by the formula



wherein in L_{A66} : R = H, and R^A = H, in L_{A67} : R = H, and R^A = CH₃, in L_{A68} : R = H, and R^A = CD₃, in L_{A69} : R = CH₃, and R^A = H, in L_{A70} : R = CD₃, and R^A = H, in L_{A71} : R = CH₃, and R^A = CH₃, in L_{A72} : R = CD₃, and R^A = CD₃, in L_{A73} : R = Ethyl, and R^A = CH₃, in L_{A74} : R = Ethyl, and R^A = CH₃, in L_{A75} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A76} : R = isopropyl, and R^A = H, in L_{A76} : R = isopropyl, and R^A = CH₃, in L_{A78} : R = isopropyl-*d7*, and R^A = CD₃, L_{A92} through L_{A104} , each represented by the formula





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$$\label{eq:constraint} \begin{split} & \text{wherein in } L_{A131}\text{: } R = \text{H, and } R^{\text{A}} = \text{H,} \\ & \text{in } L_{A132}\text{: } R = \text{H, and } R^{\text{A}} = \text{CH}_3, \\ & \text{in } L_{A133}\text{: } R = \text{H, and } R^{\text{A}} = \text{CD}_3, \end{split}$$



wherein in L _{A92} : R = H, and R ^A = H,
in L_{A93} : R = H, and R ^A = CH ₃ ,
in L_{A94} : R = H, and R ^A = CD ₃ ,
in L_{A95} : R = CH ₃ , and R ^A = H,
in L_{A96} : R = CD ₃ , and R ^A = H,
in L_{A97} : R = CH ₃ , and R ^A = CH ₃ ,
in L_{A98} : R = CD ₃ , and R ^A = CD ₃ ,
in L _{A99} : R = Ethyl, and R ^A = H,
in L_{A100} : R = Ethyl, and R ^A = CH ₃ ,
in L_{A101} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
in L _{A102:} R = isopropyl, and R ^A = H,
in L_{A103} : R = isopropyl, and R ^A = CH ₃ ,
in L_{A104} : R = isopropyl-d7, and R ^A = CD ₃ ,
L_{A118} through $L_{A130},$ each represented by the formula
••



wherein in L_{A118} : R = H, and R^A = H, in L_{A119} : R = H, and R^A = CH₃, in L_{A120} : R = H, and R^A = CD₃, in L_{A121} : R = CH₃, and R^A = H, in L_{A122} : R = CD₃, and R^A = H, in L_{A123} : R = CH₃, and R^A = CH₃, in L_{A124} : R = CD₃, and R^A = CD₃, in L_{A125} : R = Ethyl, and R^A = H, in L_{A126} : R = Ethyl, and R^A = CH₃, in L_{A126} : R = Ethyl, and R^A = CH₃, in L_{A127} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A128} : R = isopropyl, and R^A = H, in L_{A129} : R = isopropyl, and R^A = CH₃, in L_{A130} : R = isopropyl-*d7*, and R^A = CD₃, L_{A144} through L_{A156} , each represented by the formula



wherein in L_{A144} : R = H, and R^A = H, in L_{A145} : R = H, and R^A = CH₃, in L_{A146} : R = H, and R^A = CD₃,

(continued)

	in L_{A134} : R = CH ₃ , and R ^A = H,
	in L_{A135} , R = CD ₃ , and R ^A = H,
5	in L_{A136} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A137} : R = CD ₃ , and R ^A = CD ₃ ,
	in L _{A138} : R = Ethyl, and R ^A = H,
	in L_{A139} : R = Ethyl, and R ^A = CH ₃ ,
	in L_{A140} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
10	in L _{A141} : R = isopropyl, and R ^A = H,
	in L_{A142} : R = isopropyl, and $R^A = CH_3$,
	in L_{A143} : R = isopropyl-d7, and R ^A = CD ₃ ,
	L_{A157} through L_{A169} , each represented by the formula

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	wherein in L _{A157} : R = H, and R ^A = H,
	in L_{A158} : R = H, and R ^A = CH ₃ ,
25	in L_{A159} : R = H, and R ^A = CD ₃ ,
	in L_{A160} : R = CH ₃ , and R ^A = H,
	in L_{A161} : R = CD ₃ , and R ^A = H,
	in L_{A162} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A163} : R = CD ₃ , and R ^A = CD ₃ ,
30	in L_{A164} : R = Ethyl, and R ^A = H,
	in L_{A165} : R = Ethyl, and R ^A = CH ₃ ,
	in L_{A166} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
	in L_{A167} : R = isopropyl, and R ^A = H,
35	in L_{A168} : R = isopropyl, and R ^A = CH ₃ ,
	in L_{A160} : R = isopropyl-d7, and R ^A = CD ₃ ,

 L_{A183} through $L_{A195},$ each represented by the formula



	wherein in L_{A183} : R = H, and R ^A = H,
	in L_{A84} : R = H, and R ^A = CH ₃ ,
	in L_{A185} : R = H, and R ^A = CD ₃ ,
50	in L_{A186} : R = CH ₃ , and R ^A = H,
	in L_{A187} : R = CD ₃ , and R ^A = H,
	in L_{A188} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A189} : R = CD ₃ , and R ^A = CD ₃ ,
55	in L_{A190} : R = Ethyl, and R ^A = H,
00	in L_{A191} : R = Ethyl, and R ^A = CH ₃ ,
	in L_{A192} : R = Ethyl-d5, and R ^A = CD ₃ ,
	in L_{A193} : R = isopropyl, and R ^A = H,

in L_{A147} : R = CH₃, and R^A = H, in L_{A148} : R = CD₃, and R^A = H, in L_{A149} : R = CH₃, and R^A = CH₃, in L_{A150} : R = CD₃, and R^A = CD₃, in L_{A151} : R = Ethyl, and R^A = H, in L_{A152} : R = Ethyl, and R^A = CH₃, in L_{A153} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A154} : R = isopropyl, and R^A = H, in L_{A155} : R = isopropyl, and R^A = CH₃, in L_{A156} : R = isopropyl-*d7*, and R^A = CD₃,

 L_{A170} through L_{A182} , each represented by the formula



wherein in L_{A170} : R = H, and R^A = H, in L_{A171} : R = H, and R^A = CH₃, in L_{A172} : R = H, and R^A = CD₃, in L_{A173} : R = CH₃, and R^A = H, in L_{A174} : R = CD₃, and R^A = H, in L_{A175} : R = CH₃, and R^A = CH₃, in L_{A176} : R = CD₃, and R^A = CD₃, in L_{A176} : R = Ethyl, and R^A = H, in L_{A178} : R = Ethyl, and R^A = CH₃, in L_{A179} : R = Ethyl, and R^A = CH₃, in L_{A179} : R = Ethyl, and R^A = CH₃, in L_{A181} : R = isopropyl, and R^A = H, in L_{A181} : R = isopropyl, and R^A = CH₃, in L_{A181} : R = isopropyl, and R^A = CH₃, in L_{A182} : R = isopropyl-*d7*, and R^A = CD₃. L_{A196} through L_{A208} , each represented by the formula



wherein in L_{A196} : R = H, and R^A = H, in L_{A197} : R = H, and R^A = CH₃, in L_{A198} : R = H, and R^A = CD₃, in L_{A199} : R = CH₃, and R^A = H, in L_{A200} : R = CD₃, and R^A = H, in L_{A201} : R = CH₃, and R^A = CH₃, in L_{A201} : R = CD₃, and R^A = CD₃, in L_{A202} : R = CD₃, and R^A = CD₃, in L_{A203} : R = Ethyl, and R^A = H, in L_{A204} : R = Ethyl, and R^A = CH₃, in L_{A205} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A206} : R = isopropyl, and R^A = H, (continued)

in L_{A194} : R = isopropyl, and R^A = CH₃,

in L_{A195} : R = isopropyl-d7, and R^A = CD₃,

 L_{A209} through L_{A221} , each represented by the formula

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15	wherein in L _{A209} : R = H, and R ^A = H,
	in L_{A210} : R = H, and R ^A = CH ₃ ,
	in L_{A211} R = H, and R^A = CD ₃ ,
	in L_{A212} : R = CH ₃ , and R ^A = H,
20	in L_{A213} : R = CD ₃ , and R ^A = H,
	in L_{A214} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A215} : R = CD ₃ , and R ^A = CD ₃ ,
	in L _{A216} : R = Ethyl, and R ^A = H,
	in L_{A217} : R = Ethyl, and $R^A = CH_3$,
25	in L_{A218} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
	in L _{A219} : R = isopropyl, and R ^A = H,
	in L_{A220} : R = isopropyl, and R ^A = CH ₃ ,
	in L_{A221} : R = isopropyl-d7, and R ^A = CD ₃ ,

in L_{A207} : R = isopropyl, and R^A = CH₃, in L_{A208} : R = isopropyl-*d*7, and R^A = CD₃, L_{A222} through L_{A234} , each represented by the formula



wherein in L_{A222} : R = H, and R^A = H, in L_{A223} : R = H, and R^A = CH₃, in L_{A224} : R = H, and R^A = CD₃, in L_{A225} : R = CH₃, and R^A = H, in L_{A226} : R = CD₃, and R^A = CH₃, in L_{A227} : R = CH₃, and R^A = CH₃, in L_{A228} : R = CD₃, and R^A = CD₃, in L_{A229} : R = Ethyl, and R^A = H, in L_{A230} : R = Ethyl, and R^A = CH₃, in L_{A231} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A232} : R = isopropyl, and R^A = H, in L_{A233} : R = isopropyl, and R^A = CH₃, in L_{A234} : R = isopropyl-*d7*, and R^A = CD₃,

 $_{30}$ L_{A235} through L_{A247}, each represented by the formula L_A



40	wherein in L _{A235} : R = H, and R ^A = H,
	in L_{A236} : R = H, and R ^A = CH ₃ ,
	in L_{A237} : R = H, and R ^A = CD ₃ ,
	in L_{A238} : R = CH ₃ , and R ^A = H,
	in L_{A239} : R = CD ₃ , and R ^A = H,
45	in L_{A240} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A241} : R = CD ₃ , and R ^A = CD ₃ ,
	in L_{A242} : R = Ethyl, and R ^A = H,
	in L _{A243} : R = Ethyl, and R ^A = CH ₃ ,
50	in L_{A244} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
	in L_{A245} : R = isopropyl, and R ^A = H,
	in L_{A246} : R = isopropyl, and R ^A = CH ₃ ,
	in L_{A247} : R = isopropyl-d7, and R ^A = CD ₃ ,
	L_{A261} through L_{A273} , each represented by the formula
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 L_{A248} through $L_{A260},$ each represented by the formula $\label{eq:La248}$



wherein in L_{A248} : R = H, and R^A = H, in L_{A249} : R = H, and R^A = CH₃, in L_{A250} : R = H, and R^A = CD₃, in L_{A251} : R = CH₃, and R^A = H, in L_{A252} : R = CD₃, and R^A = CH₃, in L_{A253} : R = CH₃, and R^A = CD₃, in L_{A254} : R = CD₃, and R^A = CD₃, in L_{A255} : R = Ethyl, and R^A = H, in L_{A256} : R = Ethyl, and R^A = CH₃, in L_{A257} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A258} : R = isopropyl, and R^A = H, in L_{A258} : R = isopropyl, and R^A = CH₃, in L_{A260} : R = isopropyl-*d7*, and R^A = CD₃, L_{A274} through L_{A286} , each represented by the formula





wherein in L_{A274} : R = H, and R^A = H, in L_{A275} : R = H, and R^A = CH₃, in L_{A276} : R = H, and R^A = CD₃, in L_{A277} : R = CH₃, and R^A = H, in L_{A278} : R = CD₃, and R^A = H, in L_{A279} : R = CH₃, and R^A = CH₃, in L_{A280} : R = CD₃, and R^A = CD₃, in L_{A281} : R = Ethyl, and R^A = H, in L_{A282} : R = Ethyl, and R^A = CH₃, in L_{A283} : R = Ethyl-*d*5, and R^A = CD₃, in L_{A284} : R = isopropyl, and R^A = H, in L_{A285} : R = isopropyl, and R^A = CH₃, in L_{A285} : R = isopropyl-*d*7, and R^A = CD₃, L_{A300} through L_{A312} , each represented by the formula



wherein in L_{A300} : R = H, and R^A = H, in L_{A301} : R = H, and R^A = CH₃, in L_{A302} : R = H, and R^A = CD₃, in L_{A303} : R = CH₃, and R^A = H, in L_{A304} : R = CD₃, and R^A = H, in L_{A305} : R = CH₃, and R^A = CH₃, in L_{A306} : R = CD₃, and R^A = CD₃, in L_{A307} : R = Ethyl, and R^A = H, in L_{A308} : R = Ethyl, and R^A = CH₃, in L_{A309} : R = Ethyl, and R^A = CH₃, in L_{A309} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A311} : R = isopropyl, and R^A = H, in L_{A311} : R = isopropyl, and R^A = CH₃, in L_{A312} : R = isopropyl-*d7*, and R^A = CD₃, L_{A326} through L_{A338} , each represented by the formula

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10	R-V-RA	R
	wherein in L _{boxe} : $B = H$ and $B^A = H$	wherein in L
	in L_{A314} : R = H, and R ^A = CH ₃ ,	in $L_{\Delta 327}$: R = H,
	in L_{A315} : R = H, and R ^A = CD ₃ ,	in L_{A328} : R = H,
15	in L_{A316} : R = CH ₃ , and R ^A = H,	in L _{A329} : R = CH
	in L_{A317} : R = CD ₃ , and R ^A = H,	in L _{A330} : R = CI
	in L_{A318} : R = CH ₃ , and R ^A = CH ₃ ,	in L _{A331} : R = CH
	in L_{A319} : R = CD ₃ , and R ^A = CD ₃ ,	in L _{A332} : R = CI
20	in L_{A320} : R = Ethyl, and R ^A = H,	in L _{A333} : R = Et
	in L_{A321} : R = Ethyl, and R ^A = CH ₃ ,	in L _{A334} : R = Et
	in L_{A322} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,	in L _{A335} : R = Et
	in L_{A323} : R = isopropyl, and R ^A = H,	in L_{A336} : R = iso
25	In L_{A324} : R = isopropyl, and R ^A = CH ₃ ,	$\ln L_{A337}: R = isc$
25	In L_{A325} : R = Isopropyi- <i>a</i> 7, and R ^A = CD ₃ ,	In L_{A338} : R = Iso
		LA352 through LA
	ſ Ŷ	
20		
30	N _V N,	
	0	
	N-X I	
	R-CRA	
35		R
	wherein in L _{A339} : R = H, and R ^A = H,	wherein in L _{A352}
	in L_{A340} : R = H, and R ^A = CH ₃ ,	in L _{A353} : R = H,
	in L_{A341} : R = H, and R ^A = CD ₃ ,	in L _{A354} : R = H,
40	in L_{A342} : R = CH ₃ , and R ^A = H,	in L _{A355} : R = Cl
	in L_{A343} : R = CD ₃ , and R ^A = H,	in L_{A356} : R = C[
	In L_{A344} : R = CH ₃ , and R ^A = CH ₃ ,	$In L_{A357}$: R = CF
	In L_{A345} : $R = CD_3$, and $R^2 = CD_3$,	$\ln L_{A358}: R = CL$
45	in L_{A346} . R = Ethyl, and R ^A = CH	in L_{A3S9} : R – Et
	in L_{A347} . R = Ethyl-d5 and R ^A = CD ₂	in L_{A360} . R = Et
	in L_{A348} . R = isopropyl, and R ^A = H.	III = A361. IX = EC
	in L_{A350} : R = isopropyl, and R ^A = CH ₂ .	$\ln L_{A362}$: R = isc
50	in L_{A351} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ ,	in L_{A364} : R = isc
00	L_{A365} through L_{A377} , each represented by the formula	L _{A378} through L ₄

R = H, and R^A = H,

in L_{A327} : R = H, and R^A = CH₃, in L_{A328} : R = H, and R^A = CD₃, in L_{A329} : R = CH₃, and R^A = H, in L_{A330} : R = CD₃, and R^A = H, in L_{A331} : R = CH₃, and R^A = CH₃, in L_{A332} : R = CD₃, and R^A = CD₃, in L_{A332} : R = Ethyl, and R^A = CH₃, in L_{A334} : R = Ethyl, and R^A = CH₃, in L_{A335} : R = Ethyl, and R^A = CH₃, in L_{A336} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A336} : R = isopropyl, and R^A = H, in L_{A337} : R = isopropyl, and R^A = CH₃, in L_{A338} : R = isopropyl-*d7*, and R^A = CD₃,

-A352 through LA364, each represented by the formula



wherein in L_{A352} : R = H, and R^A = H, in L_{A353} : R = H, and R^A = CH₃, in L_{A354} : R = H, and R^A = CD₃, in L_{A355} : R = CH₃, and R^A = H, in L_{A356} : R = CD₃, and R^A = H, in L_{A357} : R = CH₃, and R^A = CH₃, in L_{A358} : R = CD₃, and R^A = CD₃, in L_{A360} : R = Ethyl, and R^A = H, in L_{A360} : R = Ethyl, and R^A = CH₃, in L_{A361} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A362} : R = isopropyl, and R^A = H, in L_{A363} : R = isopropyl, and R^A = CD₃, in L_{A364} : R = isopropyl-*d7*, and R^A = CD₃, L_{A378} through L_{A390} , each represented by the formula



wherein in L_{A378} : R = H, and R^A = H, in L_{A379} : R = H, and R^A = CH₃, in L_{A380} : R = H, and R^A = CD₃, in L_{A381} : R = CH₃, and R^A = H, in L_{A382} : R = CD₃, and R^A = H, in L_{A383} : R = CH₃, and R^A = CH₃, in L_{A384} : R = CD₃, and R^A = CD₃, in L_{A385} : R = Ethyl, and R^A = H, in L_{A386} : R = Ethyl, and R^A = CH₃, in L_{A387} : R = Ethyl, and R^A = CH₃, in L_{A387} : R = Ethyl, and R^A = CH₃, in L_{A387} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A388} : R = isopropyl, and R^A = CH₃, in L_{A389} : R = isopropyl, and R^A = CH₃, in L_{A389} : R = isopropyl-*d7*, and R^A = CD₃, L_{A404} through L_{A416} , each represented by the formula



wherein in L_{A404} : R = H, and R^A = H, in L_{A405} : R = H, and R^A = CH₃, in L_{A406} : R = H, and R^A = CD₃, in L_{A407} : R = CH₃, and R^A = H, in L_{A408} : R = CD₃, and R^A = H, in L_{A408} : R = CD₃, and R^A = CH₃, in L_{A410} : R = CD₃, and R^A = CD₃, in L_{A410} : R = Ethyl, and R^A = H, in L_{A412} : R = Ethyl, and R^A = CH₃, in L_{A412} : R = Ethyl, and R^A = CH₃, in L_{A413} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A414} : R = isopropyl, and R^A = H, in L_{A415} : R = isopropyl, and R^A = CH₃, in L_{A416} : R = isopropyl-*d7*, and R^A = CD₃, L_{A430} through L_{A442} , each represented by the formula



5		
10		
15	wherein in L _{A469} : R = H, and R ^A = H, in L _{A470} : R = H, and R ^A = CH ₃ , in L _{A471} : R = H, and R ^A = CD ₃ , in L _{A472} : R = CH ₃ , and R ^A = H, in L _{A472} : R = CD ₂ , and R ^A = H.	i i i
20	in L_{A474} : R = CH ₃ , and R ^A = CH ₃ , in L_{A475} : R = CD ₃ , and R ^A = CD ₃ , in L_{A476} : R = Ethyl, and R ^A = H, in L_{A477} : R = Ethyl, and R ^A = CH ₃ , in L_{A477} : R = Ethyl-d5 and R ^A = CD.	i i i
25	in L_{A478} . R = EuryPao, and R ^A = OD ₃ , in L_{A479} : R = isopropyl, and R ^A = H, in L_{A480} : R = isopropyl, and R ^A = CH ₃ , in L_{A481} : R = isopropyl- <i>d</i> 7, and R ^A = CD ₃ , L_{A495} through L_{A507} , each represented by the formula	i i i L
30		
35	$R \rightarrow R^{A}$	
40	in L_{A495} : R = H, and R ^A = CH ₃ , in L_{A497} : R = H, and R ^A = CD ₃ , in L_{A497} : R = CH ₃ , and R ^A = H,	i i i
	in L_{A499} : R = CD ₃ , and R ^A = H, in L_{A500} : R = CH ₃ , and R ^A = CH ₃ , in L_{A501} : R = CD ₃ , and R ^A = CD ₃ , in L_{A501} : R = Ethyl, and R ^A = H,	i i i
45	in L_{A503} : R = Ethyl, and R ^A = CH ₃ , in L_{A504} : R = Ethyl- <i>d</i> 5, and R ^A = CD ₃ , in L_{A505} : R = isopropyl, and R ^A = H, in L_{A505} : R = isopropyl, and R ^A = CH ₂ .	i i i
50	in L_{A507} : R = isopropyl- <i>d</i> 7, and R ^A = CD ₃ , L_{A521} through L_{A533} , each represented by the formula	i



- ^

wherein in L_{A482} : R = H, and R ^A = H,
$h L_{A483}$: R = H, and R ^A = CH ₃ ,
$h L_{A484}$: R = H, and R ^A = CD ₃ ,
n L _{A485} : R = CH ₃ , and R ^A = H,
n L _{A486} : R = CD ₃ , and R ^A = H,
$h L_{A487}$: R = CH ₃ , and R ^A = CH ₃ ,
n L _{A488} : R = CD ₃ , and R ^A = CD ₃ ,
n L _{A489} : R = Ethyl, and R ^A = H,
n L _{A490} : R = Ethyl, and R ^A = CH ₃ ,
n L _{A491} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
n L _{A492} : R = isopropyl, and R ^A = H,
$h L_{A493}$: R = isopropyl, and R ^A = CH ₃ ,
L_{A494} : R = isopropyl- <i>d</i> 7, and R ^A = CD ₃ ,
$_{A508}$ through L_{A520} , each represented by the formula









wherein in L_{A534} : R = H, and R^A = H, in L_{A535} : R = H, and R^A = CH₃, in L_{A536} : R = H, and R^A = CD₃, in L_{A637} : R = CH₃, and R^A = H, in L_{A538} : R = CD₃, and R^A = H, in L_{A539} : R = CH₃, and R^A = CH₃, in L_{A540} : R = CD₃, and R^A = CD₃, in L_{A541} : R = Ethyl, and R^A = H, in L_{A542} : R = Ethyl, and R^A = CH₃, in L_{A543} : R = Ethyl, and R^A = CH₃, in L_{A543} : R = Ethyl-d5, and R^A = CD₃, in L_{A544} : R = isopropyl, and R^A = CH₃, in L_{A545} : R = isopropyl, and R^A = CH₃, in L_{A545} : R = isopropyl-d7, and R^A = CD₃,

 L_{A560} through $L_{A572},$ each represented by the formula









wherein in L_{A586} : R = H, and R^A = H, in L_{A587} : R = H, and R^A = CH₃, in L_{A588} : R = H, and R^A = CD₃, in L_{A589} : R = CH₃, and R^A = H, in L_{A590} : R = CD₃, and R^A = H, in L_{A591} : R = CH₃, and R^A = CH₃, in L_{A592} : R = CD₃, and R^A = CD₃, in L_{A592} : R = Ethyl, and R^A = H, in L_{A594} : R = Ethyl, and R^A = CH₃, in L_{A595} : R = Ethyl, and R^A = CH₃, in L_{A596} : R = Ethyl-*d*5, and R^A = CD₃, in L_{A596} : R = isopropyl, and R^A = H, in L_{A597} : R = isopropyl, and R^A = CH₃, in L_{A597} : R = isopropyl-*d*7, and R^A = CD₃, L_{A612} through L_{A624} , each represented by the formula



wherein in L _{A612} : R = H, and R ^A = H,				
in $L_{A613:} R = H$, and $R^A = CH_3$,				
in L _{A614} : R = H, and R ^A = CD ₃ ,				
in L_{A415} : R = CH ₃ , and R ^A = H,				
in L_{A616} : R = CD ₃ , and R ^A = H,				
In L_{A617} : R = CH ₃ , and R ^A = CH ₃ ,				
in L_{A618} : R = CD ₃ , and R ^A = CD ₃ ,				
in L _{A619} : R = Ethyl, and R ^A = H,				
in L_{A620} : R = Ethyl, and R ^A = CH ₃ ,				
in L_{A621} : R = Ethyl- <i>d</i> 5, and R ^A = CD ₃ ,				
n L _{A622} : R = isopropyl, and R ^A = H,				
in L_{A623} : R = isopropyl, and R ^A = CH ₃ ,				
In L_{A624} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ ,				
$L_{ m A638}$ through $L_{ m A650}$, each represented by the formula				

	(continued)		
5			
10		R RA	
15	wherein in L_{A625} : R = H, and R ^A = H, in L_{A626} : R = H, and R ^A = CH ₃ , in L_{A627} : R = H, and R ^A = CD ₃ , in L_{A628} : R = CH ₃ , and R ^A = H, in L_{A629} : R = CD ₃ , and R ^A = H, in L_{A630} : R = CH ₃ , and R ^A = CH ₃ ,	wherein in L_{A638} : R = H, and R ^A = H, in L_{A639} : R = H, and R ^A = CH ₃ , in L_{A640} : R = H, and R ^A = CD ₃ , in L_{A641} : R = CH ₃ , and R ^A = H, in L_{A642} : R = CD ₃ , and R ^A = H, in L_{A643} : R = CH ₃ , and R ^A = CH ₃ ,	
20	in L_{A631} : R = CD ₃ , and R ^A = CD ₃ , in L_{A632} : R = Ethyl, and R ^A = H, in L_{A633} : R = Ethyl, and R ^A = CH ₃ , in L_{A634} : R = Ethyl- <i>d</i> 5, and R ^A = CD ₃ ,	in L_{A644} : R = CD ₃ , and R ^A = CD ₃ , in L_{A645} : R = Ethyl, and R ^A = H, in L_{A646} : R = Ethyl, and R ^A = CH ₃ , in L_{A647} : R = Ethyl- <i>d</i> 5, and R ^A = CD ₃ ,	
25	in L_{A635} : R = isopropyl, and R ^A = H, in L_{A636} : R = isopropyl, and R ^A = CH ₃ , in L_{A637} : R = isopropyl- <i>d</i> 7, and R ^A = CD ₃ , L_{A651} through L_{A663} , each represented by the formula	in L _{A648} : R = isopropyl, and R ^A = H, in L _{A649} : R = isopropyl, and R ^A = CH ₃ , in L _{A650} : R = isopropyl- <i>d</i> 7, and R ^A = CD ₃ , L _{A664} through L _{A676} , each represented by the formula	
30 35	R-N-RA R-RA		
40	wherein in L_{A651} : R = H, and R ^A = H, in L_{A652} : R = H, and R ^A = CH ₃ , in L_{A653} : R = H, and R ^A = CD ₃ , in L_{A654} : R = CH ₃ , and R ^A = H, in L_{A655} : R = CD ₃ , and R ^A = H, in L_{A655} : R = CD ₃ , and R ^A = H,	wherein in L_{A664} : R = H, and R ^A = H, in L_{A665} : R = H, and R ^A = CH ₃ , in L_{A666} : R = H, and R ^A = CD ₃ , in L_{A667} : R = CH ₃ , and R ^A = H, in L_{A668} : R = CD ₃ , and R ^A = H, in L_{A668} : R = CH ₂ , and R ^A = CH ₂ .	
45	in L_{A656} : R = CD ₃ , and R ^A = CD ₃ , in L_{A657} : R = CD ₃ , and R ^A = CD ₃ , in L_{A659} : R = Ethyl, and R ^A = H, in L_{A660} : R = Ethyl- <i>d</i> 5, and R ^A = CD ₃ , in L_{A661} : R = isopropyl, and R ^A = H,	in L_{A663} : R = CD ₃ , and R ^A = CD ₃ , in L_{A671} : R = Ethyl, and R ^A = CD ₃ , in L_{A672} : R = Ethyl, and R ^A = CH ₃ , in L_{A673} : R = Ethyl- <i>d</i> 5, and R ^A = CD ₃ , in L_{A674} : R = isopropyl, and R ^A = H,	
50	in L_{A662} : R = isopropyl, and R ^A = CH ₃ , in L_{A663} : R = isopropyl- <i>d</i> 7, and R ^A = CD ₃ , L_{A677} through L_{A689} , each represented by the formula	in L_{A675} : R = isopropyl, and R ^A = CH ₃ , in L_{A676} : R = isopropyl- <i>d</i> 7, and R ^A = CD ₃ , L_{A690} through L_{A702} , each represented by the formula	





wherein in L_{A690} : R = H, and R^A = H, in L_{A691} : R = H, and R^A = CH₃, in L_{A692} : R = H, and R^A = CD₃, in L_{A693} : R = CH₃, and R^A = H, in L_{A694} : R = CD₃, and R^A = H, in L_{A695} : R = CH₃, and R^A = CH₃, in L_{A696} : R = CD₃, and R^A = CD₃, in L_{A697} : R = Ethyl, and R^A = CH₃, in L_{A699} : R = Ethyl, and R^A = CH₃, in L_{A699} : R = Ethyl-d5, and R^A = CD₃, in L_{A699} : R = isopropyl, and R^A = H, in L_{A700} : R = isopropyl, and R^A = CH₃, in L_{A701} : R = isopropyl-d7, and R^A = CD3, and

 $[0060] \quad \mbox{In some specific embodiments, } L_C \mbox{ is selected from the group consisting of:}$



 $[0061] \quad \mbox{In some embodiments, } L_B \mbox{ is selected from the group consisting of:}$



[0062] In some specific embodiments, the compound is selected from the group consisting of:













[0063] According to another aspect of the present disclosure, a first device is also provided. The first device includes a first organic light emitting device, that includes an anode, a cathode, and an organic layer disposed between the anode and the cathode. The organic layer may include a host and a phosphorescent dopant. The organic layer can include a compound according to Formula $M(L_A)_x(L_B)_y(L_C)_z$, and its variations as described herein.

[0064] The first device can be one or more of a consumer product, an organic light-emitting device and a lighting panel. The organic layer can be an emissive layer and the compound can be an emissive dopant in some embodiments, while the compound can be a non-emissive dopant in other embodiments.

- [0065] The organic layer can also include a host. In some embodiments, the host can include a metal complex. The
- ⁵ host can be a triphenylene containing benzo-fused thiophene or benzo-fused furan. Any substituent in the host can be an unfused substituent independently selected from the group consisting of C_nH_{2n+1} , OC_nH_{2n+1} , OAr_1 , $N(C_nH_{2n+1})_2$, $N(Ar_1)(Ar_2)$, $CH=CH-Cl_nH_{2n+1}$, $C\equiv C-C_nH_{2n+1}$, Ar_1 , Ar_1-Ar_2 , $C_nH_{2n}-Ar_1$, or no substitution. In the preceding substituents n can range from 1 to 10; and Ar_1 and Ar_2 can be independently selected from the group consisting of benzene, biphenyl, naphthalene, triphenylene, carbazole, and heteroaromatic analogs thereof.
- ¹⁰ **[0066]** The host can be a compound selected from the group consisting of carbazole, dibenzothiphene, dibenzofuran, dibenzoselenophene, azacarbazole, aza-dibenzothiphene, aza-dibenzofuran, and aza-dibenzoselenophene. The host can include a metal complex. The host can be a specific compound selected from the group consisting of:





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and combinations thereof.

[0067] In yet another aspect of the present disclosure, a formulation that comprises a compound according to Formula $M(L_A)_x(L_B)_y(L_C)_z$ is described. The formulation can include one or more components selected from the group consisting of a solvent, a host, a hole injection material, hole transport material, and an electron transport layer material, disclosed herein.

15 here

COMBINATION WITH OTHER MATERIALS

[0068] The materials described herein as useful for a particular layer in an organic light emitting device may be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used in conjunction with a wide variety of hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

HIL/HTL:

[0069] A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but not limit to: a phthalocyanine or porphyrin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly monomer derived from compounds such as phosphonic acid and silane derivatives; a metal oxide derivative, such as MoO_x; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

35 [0070] Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:





chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimi-

- ⁵ dazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly
- ¹⁰ or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each Ar is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.
- ¹⁵ **[0072]** In one aspect, Ar¹ to Ar⁹ is independently selected from the group consisting of:



³⁰ wherein k is an integer from 1 to 20; X¹⁰¹ to X¹⁰⁸ is C (including CH) or N; Z¹⁰¹ is NAr¹, O, or S; Ar¹ has the same group defined above.

[0073] Examples of metal complexes used in HIL or HTL include, but not limit to the following general formula:

35

$$\begin{bmatrix} (Y^{101}) \\ Y^{102} \\ k' \end{bmatrix} Met - (L^{101})k''$$

40 wherein Met is a metal, which can have an atomic weight greater than 40; (Y¹⁰¹-Y¹⁰²) is a bidentate ligand, Y¹⁰¹ and Y¹⁰² are independently selected from C, N, O, P, and S; L¹⁰¹ is an ancillary ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

[0074] In one aspect, (Y¹⁰¹-Y¹⁰²) is a 2-phenylpyridine derivative. In another aspect, (Y¹⁰¹-Y¹⁰²) is a carbene ligand.
 In another aspect, Met is selected from Ir, Pt, Os, and Zn. In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc⁺/Fc couple less than about 0.6 V.

Host:

- 50 [0075] The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant. While the Table below categorizes host materials as preferred for devices that emit various colors, any host material may be used with any dopant so long as the triplet
- ⁵⁵ criteria is satisfied.

[0076] Examples of metal complexes used as host are preferred to have the following general formula:

$$\begin{bmatrix} (Y^{103}) \\ (Y^{104}) \\ k' \end{bmatrix}$$
Met — (L¹⁰¹)k"

15

wherein Met is a metal; $(Y^{103}-Y^{104})$ is a bidentate ligand, Y^{103} and Y^{104} are independently selected from C, N, O, P, and S; L^{101} is an another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

¹⁰ [0077] In one aspect, the metal complexes are:

$$\begin{bmatrix} \begin{pmatrix} 0 \\ N \end{bmatrix}_{k'}^{AI-(L^{101})_{3\cdot k'}} \begin{bmatrix} \begin{pmatrix} 0 \\ N \end{bmatrix}_{k'}^{Zn-(L^{101})_{2\cdot k'}} \end{bmatrix}$$

wherein (O-N) is a bidentate ligand, having metal coordinated to atoms O and N.

[0078] In another aspect, Met is selected from Ir and Pt. In a further aspect, $(Y^{103}-Y^{104})$ is a carbene ligand.

- 20 [0079] Examples of organic compounds used as host are selected from the group consisting aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenan-threne, fluorene, pyrene, chrysene, perylene, azulene; group consisting aromatic heterocyclic compounds such as diben-zothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole,
- oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and group consisting 2 to 10 cyclic structural units which are groups of the same type or different
- types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Wherein each group is further substituted by a substituent selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfanyl, sulfonyl, phosphino, and combinations thereof.
- [0080] In one aspect, host compound contains at least one of the following groups in the molecule:



50



wherein R¹⁰¹ to R¹⁰⁷ is independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl,
 heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl,
 carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when
 it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above. k is an integer from 0 to 20 or 1 to 20; k''' is
 an integer from 0 to 20. X¹⁰¹ to X¹⁰⁸ is selected from C (including CH) or N.
 Z¹⁰¹ and Z¹⁰² is selected from NR¹⁰¹, O, or S.

25 HBL:

[0081] A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED.

[0082] In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

[0083] In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

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wherein k is an integer from 1 to 20; L¹⁰¹ is an another ligand, k' is an integer from 1 to 3.

45 ETL:

[0084] Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

[0085] In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

55


wherein R¹⁰¹ is selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above. Ar¹ to Ar³ has the similar definition as Ar's mentioned above. k is an integer from 1 to 20. X¹⁰¹ to X¹⁰⁸ is selected from C (including CH) or N.

[0086] In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:

25

20

$$\left[\left(\begin{array}{c}0\\N\end{array}\right)_{k'}^{AI-(L^{101})_{3\cdot k'}}\left[\left(\begin{array}{c}0\\N\end{array}\right)_{k'}^{Be-(L^{101})_{2\cdot k'}}\left[\left(\begin{array}{c}0\\N\end{array}\right)_{k'}^{Zn-(L^{101})_{2\cdot k'}}\left[\left(\begin{array}{c}0\\N\end{array}\right)_{k'}^{Zn-(L^{101})_{2\cdot k'}}\right]\right]\right]$$

30

35

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wherein (O-N) or (N-N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L¹⁰¹ is another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

[0087] In any above-mentioned compounds used in each layer of the OLED device, the hydrogen atoms can be partially or fully deuterated. Thus, any specifically listed substituent, such as, without limitation, methyl, phenyl, pyridyl, etc. encompasses undeuterated, partially deuterated, and fully deuterated versions thereof. Similarly, classes of substituents such as, without limitation, alkyl, aryl, cycloalkyl, heteroaryl, etc. also encompass undeuterated, partially deuterated, and fully deuterated, and fully deuterated, partially deuterated.

[0088] In addition to and / or in combination with the materials disclosed herein, many hole injection materials, hole transporting materials, host materials, dopant materials, exiton/hole blocking layer materials, electron transporting and electron injecting materials may be used in an OLED. Non-limiting examples of the materials that may be used in an OLED in combination with materials disclosed herein are listed in Table 1 below. Table 1 lists non-limiting classes of materials, non-limiting examples of compounds for each class, and references that disclose the materials.

15	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS	
	Hole injection materials			
50	Phthalocyanine and porphryin compounds		Appl. Phys. Lett. 69, 2160 (1996)	

TABL	E 1
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	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	Starburst triarylamines		J. Lumin. 72-74, 985 (1997)
10			
15	CF _X Fluorohydrocarbon polymer	CH _x F _y	Appl. Phys. Lett. 78, 673 (2001)
20	Conducting polymers (e.g., PEDOT:PSS, polyaniline, polypthiophene)	$ \begin{bmatrix} & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & &$	Synth. Met. 87, 171 (1997) WO2007002683
25	Phosphonic acid and silane SAMs		US20030162053
30	Triarylamine or polythiophene polymers with conductivity dopants		EP1725079A1
35			
40		⋤ <mark>∊</mark> ₽ [⋫] ⋎ <u></u> ҇⋤ ₽ ⋶⋌⋺ <mark>─</mark> ₿─⋌⋺ ⋶⋝ <mark>⋶</mark> ⋤ ₽	
45	Organic compounds with conductive inorganic compounds, such as molybdenum and tungsten oxides		US20050123751 SID Symposium Digest, 37, 923 (2006) WO2009018009
50	n-type semiconducting organic complexes		US20020158242
55			

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Metal organometallic complexes		US20060240279
Cross-linkable compounds		US20080220265
Polythiophene based polymers and copolymers		WO 2011075644 EP2350216
Hole transporting materials		
Triarylamines (e.g., TPD, α- NPD)		Appl. Phys. Lett. 51, 913 (1987)
		US5061569

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5			EP650955
10			
15			J. Mater. Chem. 3, 319 (1993)
20			
25			Appl. Phys. Lett. 90, 183503 (2007)
30 35			Appl. Phys. Lett. 90, 183503 (2007)
40	Triaylamine on spirofluorene core	Ph ₂ N-V-NPh ₂ Ph ₂ N-V-NPh ₂	Synth. Met. 91, 209 (1997)
45	Arylamine carbazole compounds		Adv. Mater. 6, 677 (1994), US20080124572
50			
55	Triarylamine with (di)benzothiophene/(di)ben zofuran		US20070278938, US20080106190 US20110163302

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	Indolocarbazoles		Synth. Met. 111, 421 (2000)
10			
	Isoindole compounds		Chem. Mater. 15, 3148 (2003)
15			
20	Metal carbene complexes		US20080018221
25			
	Phosphorescent OLED host materials		
30	Red hosts		
	Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
35	Metal 8-hydroxyquinolates (e.g., Alq ₃ , BAlq)		Nature 395, 151 (1998)
40			US20060202194
45			WO2005014551
50			WO2006072002
55	Metal phenoxybenzothiazole compounds		Appl. Phys. Lett. 90, 123509 (2007)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	Conjugated oligomers and polymers (e.g., polyfluorene)	C ₈ H ₁₇ C ₈ H ₁₇	Org. Electron. 1, 15 (2000)
10	Aromatic fused rings		WO2009066779, WO2009066778, WO2009063833, US20090045731, US20090045730, WO2009008311, US20090008605, US20090009065
20	Zinc complexes		WO2010056066
25	Chrysene based compounds		WO2011086863
30	Green hosts		
	Arylcarbazoles		Appl. Phys. Lett. 78, 1622 (2001)
35			US20030175553
40			WO2001039234
45 50	Aryltriphenylene compounds		US20060280965
55			US20060280965

(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		WO2009021126
Poly-fused heteroaryl compounds		US20090309488 US20090302743 US20100012931
Donor acceptor type molecules		WO2008056746
	N N N	
		WO201010107244
Aza-carbazole/DBT/DBF	F F	JP2008074939
		US20100187984

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	Polymers (e.g., PVK)		Appl. Phys. Lett. 77, 2280 (2000)
10	Spirofluorene compounds	J. J.	WO2004093207
15	Metal phenoxybenzooxazole compounds		WO2005089025
20			WO2006132173
25		$\begin{bmatrix} 0 & N \\ 0 & -0 \end{bmatrix}_2^{Zn}$	JP200511610
35	Spirofluorene-carbazole compounds	J-0-20-0-J	JP2007254297
40			JP2007254297
45	Indolocarbazoles		WO2007063796
50			WO2007063754
55	1		

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	5-member ring electron deficient heterocycles (e.g., triazole, oxadiazole)		J. Appl. Phys. 90, 5048 (2001)
10			WO2004107822
15 20	Tetraphenylene complexes		US20050112407
25	Metal phenoxypyridine compounds		WO2005030900
30 35	Metal coordination complexes (e.g., Zn, Al with N^N ligands)	Zn 2	US20040137268, US20040137267
	Blue hosts		
40	Arylcarbazoles		Appl. Phys. Lett, 82, 2422 (2003)
45			US20070190359
50	Dibenzothiophene/Dibenz ofuran-carbazole compounds		WO2006114966, US20090167162

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5			US20090167162
15			WO2009086028
20			US20090030202, US20090017330
25			US20100084966
30 35	Silicon aryl compounds		US20050238919
40			WO2009003898
45	Silicon/Germanium aryl compounds		EP2034538A
55	Aryl benzoyl ester		WO2006100298

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	Carbazole linked by non- conjugated groups		US20040115476
10	Aza-carbazoles		US20060121308
15 20	High triplet metal organometallic complex		US7154114
	Phosphorescent dopants		
	Red dopants		
25	Heavy metal porphyrins (e.g., PtOEP)		Nature 395, 151 (1998)
30		, , , , , , , , , , , , , , , , , , ,	

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	Iridium(III) organometallic complexes		Appl. Phys. Lett. 78, 1622 (2001)
10			US20030072964
15 20			US20030072964
25			US20060202194
30			US20060202194
35			US20070087321
40 45			US20080261076 US20100090591
50			US20070087321
55		H ₁₇ C ₈	Adv. Mater. 19, 739 (2007)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5 10		Ir(acac)	WO2009100991
15 20			WO2008101842
25		PPh ₃ Ir-Cl PPh ₃	US7232618
30	Platinum(II) organometallic complexes		WO2003040257
35			US20070103060
40			
45	Osminum(III) complexes	$\begin{bmatrix} F_{3}C \\ N \\ N \\ N \\ 2 \end{bmatrix}_{2}^{N} Os(PPhMe_{2})_{2}$	Chem. Mater. 17, 3532 (2005)
50	Ruthenium(II) complexes		Adv. Mater. 17, 1059 (2005)
55	Rhenium (I), (II), and (III) complexes	Re-(CO) ₄	US20050244673

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Green dopants	· · · · · · · · · · · · · · · · · · ·	-
Iridium(III) organometallic complexes	and its derivatives	Inorg. Chem. 40, 1704 (2001
		US20020034656
		US7332232
		US20090108737

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5			WO2010028151
10			
15 20			EP1841834B
25			US20060127696
30			US20090039776
40			US6921915
45			US20100244004
50			US6687266

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5			Chem. Mater. 16, 2480 (2004)
10			US20070190359
15			US 20060008670 JP2007123392
20 25			WO2010086089, WO2011044988
30			Adv. Mater. 16, 2003 (2004)
35			Angew. Chem. Int. Ed. 2006,45,7800
40			WO2009050290
45			US20090165846
50			US20080015355
55			

(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
	$\begin{bmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	US20010015432
		US20100295032
Monomer for polymeric metal organometallic compounds		US7250226, US7396598
Pt(II) organometallic complexes, including polydentated ligands		Appl. Phys. Lett. 86, 153505 (2005)
		Appl. Phys. Lett. 86, 153505 (2005)
		Chem. Lett. 34, 592 (2005)
		WO2002015645
	Ph Ph	US20060263635

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MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
		US20060182992 US20070103060
	Pt	
Cu complexes		WO2009000673
	\bigcirc	US20070111026
	(iBu) ₂ P N P(iBu) ₂	
	(iBu) ₂ P N P(iBu) ₂	
Gold complexes		Chem. Commun. 2906 (2005)
Rhenium(III) complexes	CF ₃	Inorg. Chem. 42, 1248 (2003)
	F ₃ C N OC Re OC C	
Osmium(II) complexes		US7279704
	N	
	Os	

(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Deuterated organometallic complexes	$\begin{bmatrix} D \\ D $	US20030138657
Organometallic complexes with two or more metal centers		US20030152802
	F N N N N N N N N N N N N N N N N N N N	US7090928

(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Iridium(III) organometallic complexes		WO2002002714
		WO2006009024
		US20060251923 US20110057559 US20110204333
		US7393599, WO2006056418, US20050260441, WO2005019373
		US7534505

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5		$\begin{bmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	WO2011051404
15			US7445855
20 25			US20070190359, US20080297033 US20100148663
30 35			US7338722
40			US20020134984
<i>45</i> 50		$\begin{bmatrix} & & & \\ & & & & \\ & & & \\ & & $	Angew. Chem. Int. Ed. 47, 4542 (2008)
55			Chem. Mater. 18, 5119 (2006)

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5			Inorg. Chem. 46, 4308 (2007)
10 15			WO2005123873
20			WO2005123873
25			WO2007004380
30			WO2006082742
35	Osmium(II) complexes		US7279704
45		$\begin{bmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Organometallics 23, 3745 (2004)
	Gold complexes	Ph ₂ P PPh ₂ CI Au Au	Appl. Phys. Lett.74,1361 (1999)
50	Platinum(II) complexes	S N-N, N N-N, N N-N, N N-N N-N	WO2006098120, WO2006103874

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	Pt tetradentate complexes with at least one metal-carbene bond		US7655323
	Exciton/hole blocking layer m	aterials	
15	Bathocuprine compounds (e.g., BCP, BPhen)		Appl. Phys. Lett. 75, 4 (1999)
20			Appl. Phys. Lett. 79, 449 (2001)
25	Metal 8-hydroxyquinolates (e.g., BAlq)		Appl. Phys. Lett. 81, 162 (2002)
30	5-member ring electron deficient heterocycles such as triazole, oxadiazole, imidazole, benzoimidazole		Appl. Phys. Lett. 81, 162 (2002)
35 40	Triphenylene compounds		US20050025993
45 50	Fluorinated aromatic compounds	$F \rightarrow F \qquad F \rightarrow F \rightarrow$	Appl. Phys. Lett. 79, 156 (2001)

(continued)

MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
Phenothiazine-S-oxide		WO2008132085
Silylated five-membered nitrogen, oxygen, sulfur or phosphorus dibenzoheterocycles		WO2010079051
Aza-carbazoles		US20060121308
Electron transporting materi	als	
Anthracene-benzoimidazole compounds		WO2003060956
		US20090179554
Aza triphenylene derivatives		US20090115316
Anthracene-benzothiazole compounds		Appl. Phys. Lett. 89, 063504 (2006)
Metal 8-hydroxyquinolates (e.g., Alq ₃ , Zrq ₄)		Appl. Phys. Lett. 51, 913(1987) US7230107

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	Metal hydroxybenoquinolates	E Be	Chem. Lett. 5, 905 (1993)
0	Bathocuprine compounds such as BCP, BPhen, etc		Appl. Phys. Lett. 91, 263503 (2007)
5			Appl. Phys. Lett. 79, 449 (2001)
0	5-member ring electron deficient heterocycles (e.g.,triazole, oxadiazole, imidazole, benzoimidazole)		Appl. Phys. Lett. 74, 865 (1999)
5			
0		C C C C C	Appl. Phys. Lett. 55, 1489 (1989)
5		N-N N-N C	Jpn. J. Apply. Phys. 32, L917 (1993)
0	Silole compounds		Org. Electron. 4, 113 (2003)
5	Arylborane compounds		J. Am. Chem. Soc. 120, 9714 (1998)
0	Fluorinated aromatic compounds	$F \xrightarrow{F}_{F} \xrightarrow{F}} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F}_{F} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F} \xrightarrow{F}} \xrightarrow{F} \xrightarrow{F}} \mathsf{$	J. Am. Chem. Soc. 122, 1832 (2000)

(continued)

	MATERIAL	EXAMPLES OF MATERIAL	PUBLICATIONS
5	Fullerene (e.g., C60)		US20090101870
15	Triazine complexes		US20040036077
20			
25	Zn (N^N) complexes	Zn SO ₂ 2	US6528187

30 EXPERIMENTAL

Synthetic Examples

[0089] All reactions were carried out under nitrogen protections unless specified otherwise. All solvents for reactions are anhydrous and used as received from commercial sources.

Synthesis of 8-(isoquinolin-1-yl)-2-methylbenzofuro[2,3-b]pyridine

[0090]

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[0091] 2-methyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzofuro[2,3-b]pyridine (4.73 g, 15.3 mmol), 1-chlo roisoquinoline (2.75 g, 16.8 mmol), Pd₂dba₃ (0.28 g, 0.31 mmol), SPhos (0.50 g, 1.22 mmol), and K₃PO₄.H₂O (10.6 g, 45.9 mmol) were dissolved in toluene (170 mL) and Water (20 mL), degassed by bubbling nitrogen, and heated to 100°C overnight. Upon completion of the reaction, the reaction mixture was cooled to room temperature and extracted with toluene. The crude material was purified via column chromatography using 20% ethyl acetate in 80% heptanes. It was noticed that a lot of deborylated compound was collected. After most of the impurity had come out, the mobile phase
was gradually increased to 40% ethyl acetate in heptanes. The material was recrystallized from methanol to obtain the pure product, 8-(isoquinolin-1-yl)-2-methylbenzofuro[2,3-b]pyridine (0.60 g, 13 % yield).

Synthesis of Compound 10

[0092]



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[0093] The Ir(III) intermediate shown above, left, (0.510 g, 0.687 mmol) and 8-(isoquinolin-1-yl)-2-methylbenzofuro[2,3b]pyridine (0.640 g, 2.062 mmol) were mixed in 7 mL of ethanol and heated to reflux for 36 hours. The reaction was stopped when there was no Ir timer left as shown by HPLC. The mixture was cooled to room temperature and filtered through a pad of Celite. The solid was collected by washing the Celite pad with dichloromethane (DCM). The crude material was purified by column chromatography starting with 50% DCM in heptanes and gradually increasing to 80% DCM in heptanes. The red solid product, compound 10, was collected (0.40 g, 70% yield).

Synthesis of Compound 24

Synthesis of 8-(5-chroroquinolin-2-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine

[0094]



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[0095] 2,6-dimethyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzofuro[2,3-b]pyridine (7.0 g, 21.7 mmol), 2,5dichloroquinoline (4.50 g, 22.7 mmol), and K₂CO₃ (5.99 g, 43.3 mmol) were dissolved in toluene (180 mL) and water (36 mL). The mixture was degassed by bubbling with nitrogen for 15 minutes, then $Pd(PPh_{3})_{4}$ (1.25 g, 1.08 mmol) was added and the mixture was heated to reflux overnight. Upon completion, the mixture was cooled to room temperature, extracted using ethyl acetate, and the organic layer was washed with brine ansd water. The crude mixture was filtered through a plug of silica using a dichloromethane and ethyl acetate mixture. After evaporation of the solvent, the product was triturated from heptanes to yield pure 8-(5-chloroquinolin-2-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (6.0 g, 77% yield).

50 Synthesis of 8-(5-isobutylquinolin-2-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine

[0096]



[0097] 8-(5-chloroquinolin-2-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (4.75 g, 13.2 mmol), isobutylboronic acid (2.70 g, 26.5 mmol), Pd₂dba₃ (0.24 g, 0.27 mmol),dicyclohexyl(2',6'-dimethoxy-[1,1'-biphenyl]-2-yl)phosphine (SPhos) (0.44 g, 1.06 mmol), and K₃PO₄ (5.62 g, 26.5 mmol) were dissolved in toluene (150 mL) and water (15 mL). The solution was degassed by bubbling nitrogen for 15 minutes, then refluxed overnight. Upon completion, the mixture was cooled to room temperature, extracted using ethyl acetate, and washed with water. The crude product was purified by column chromatography using 25% ethyl acetate in heptanes. The product was further purified by recrystallization from heptanes to yield 8-(5-isobutylquinolin-2-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (4.5 g, 89% yield)



[0098]



45

[0099] 8-(5-isobutylquinolin-2-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (3.00 g, 7.88 mmol) was solubilized in ethoxyethanol (25 mL) and water (8 mL), then degassed by bubbling nitrogen for 30 minutes. Iridium chloride (0.97 g, 2.63 mmol) was then added to the solution and the reaction was refluxed under nitrogen for 24h. After cooling to room temperature, the solid was filtered, washed with methanol, and dried to give the Ir(III) Dimer (1.95 g, 0.99 mmol, 75 % yield) as a light orange powder.

Synthesis of Compound 24.

[0100]

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[0101] Ir(III) dimer (0.39 g, 0.20 mmol) and 3,7-diethylnonane-4,6-dione (0.42 g, 1.98 mmol) were added to a flask. The mixture was diluted in ethoxyethanol (6.6 mL) and degassed by bubbling nitrogen for 15 minutes. K₂CO₃ (0.27 g, 1.98 mmol) was then added to the mixture, which was then stirred at room temperature overnight. Upon completion of the reaction, the mixture was diluted in dichloromethane (DCM), filtered through a pad of Celite, and washed with more DCM. The solvents were evaporated and the crude material was purified by column chromatography using triethylamine (TEA) pre-treated silica gel. The mobile phase used was 10% DCM in heptanes. The resulting product - Compound 24 - was purified by recrystallization from a DCM and methanol mixture to afford 0.2 g (44% yield).

25 Synthesis of Compound 44

Synthesis of 8-(6-chroroisoquinolin-1-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine

[0102]

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[0103] 1,6-dichloroisoquinoline (4.80 g, 24.2 mmol), 2,6-dimethyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ben-zofuro[2,3-b]pyridine (8.22 g, 25.4 mmol), sodium carbonate (6.42 g, 60.6 mmol), palladium tetrakis (0.84 g, 0.73 mmol), 160 mL dimethoxyethane (DME) and 40 mL of water were combined in a round bottom flask. A condenser was attached and then the system was evacuated and purged with nitrogen three times. The reaction mixture was heated to a vigorous reflux overnight. The reaction mixture was diluted with ethyl acetate and water, the suspension was then filtered through Celite and washed with ethyl acetate. The aqueous portion was partitioned off and the organic was washed once with brine, dried with sodium sulfate, filtered, and concentrated down to beige solid. The Celite was further washed with 50/50 DCM/THF and the filtrate was concentrated and combined with the other crude sample. The combined crude sample was dissolved in DCM and purified with silica gel using DCM to 85/15 DCM/ethyl acetate solvent system to get a pale beige solid. The pale beige solid was triturated in 90/10 heptane/ethyl acetate, then filtered to get a white precipitate of 8-(6-chloroisoquinolin-1-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (7.8 g, 91% yield).

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 $\underline{Synthesis \ of \ 8-(6-isopropylisoquinolin-1-yl)-2, 6-dimethylbenzofuro[2,3-b] pyridine}$

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[0104]



[0105] 8-(6-chloroisoquinolin-1-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (4.0 g, 11.2 mmol), 2'-(dicyclohexylphosphino)-N2,N2,N6,N6-tetramethyl-[1,1'-biphenyl]-2,6-diamine (0.39 g, 0.89 mmol), diacetoxypalladium (0.10 g, 0.45 mmol) and 200 ml anhydrous THF were combined in an oven dried three neck round bottom flask. A condenser was attached then the system was evacuated and purged with nitrogen three times. The reaction was heated to 60° for 15 min to dissolve the reactant and form the catalyst to get a pale brown solution. The reaction was then cooled to 0°C, then isopropylzinc(II) bromide (33 mL, 16.7 mmol) was added rapidly with a syringe through a septum. The reaction mixture

- was allowed to stir in the ice bath for 30 minutes then removed to let it warm to room temperature. Upon completion of the reaction, it was quenched with ammonium chloride solution then filtered through a Celite plug. The Celite was washed well with ethyl acetate. The aqueous portion was partitioned off and the organic portion was washed once with brine, dried with sodium sulfate, filtered, and then concentrated down to yield 5.5 g of a brown solid. The brown solid was dissolved in DCM and purified with a silica gel cartridge using a DCM to 85/15 DCM/EtOac solvent system to get 3.8 g of an off-white sticky solid. The sample was dissolved in acetonitrile and purified with C18 cartridges using a 50/50 to 85/15 acetonitrile/water solvent system. This produced 1.3 g of pure white solid. The crude fraction were re-purified
- ²⁵ using the same technique to produce 2.2 g (54% yield) of 8-(6-isopropylisoquinolin-1-yl)-2, 6-dimethylbenzofuro[2,3-b]pyridine, the pure target compound.

Synthesis of Ir(III) Dimer

30 [0106]

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[0107] 8-(6-isopropylisoquinolin-1-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (2.5 g, 6.82 mmol) was solubilized in ethoxyethanol (19 mL) and water (6 mL), then degassed with nitrogen for 30 minutes. Iridium chloride (0.56 g, 1.52 mmol) was then added to the solution and the reaction mixture was refluxed under nitrogen for 24 hours. After cooling to room temperature, the solid was filtered, washed with methanol, and dried to give Ir (III) Dimer (1.9 g, 0.99 mmol, 131 % yield) as a brown powder. The yield was higher than 100% because of the ligand remaining within the solid. The solid was used as is.

Synthesis of Compound 44

55 **[0108]**



15 [0109] The Ir(III) Dimer (1.22 g, 0.78 mmol) and 3,7-diethylnonane-4,6-dione (1.66 g, 7.84 mmol) were solubilized in 2-ethoxyethanol (26 mL) and degassed by bubbling nitrogen for 15 minutes. Potassium carbonate (1.08 g, 7.84 mmol) was then added and the mixture was stirred at room temperature overnight. The dimer was not completely consumed, so the mixture was then heated to 50 °C for 4 hours. Upon completion, the mixture was diluted in DCM and filtered through a pad of Celite, then washed with DCM. The solvents were evaporated and the crude material was purified by column chromatography (pre-treated with triethylamine) starting from 10% DCM in Heptanes to 40% DCM in Heptanes. The dark red solid weas recrystallized from a mixture of DCM and methanol to yield the pure product, Compound 44 (1.4g, 63% yield).

Synthesis of Compound 56

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Synthesis of 8-(7-chloroquinazolin-4-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine

[0110]







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[0111] 4,7-dichloroquinazoline (3.00 g, 15.1 mmol) and 2,6-dimethyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2yl)benzofuro[2,3-b]pyridine (5.11 g, 15.8 mmol), and K_2CO_3 (4.17 g, 30.1 mmol) were dissolved in DME (150 mL) and Water (40 mL). The solution was degassed by bubbling nitrogen gas, Pd(PPh₃)₄ (0.70 g, 0.60 mmol) was added and the reaction was heated to reflux overnight. Upon completion of the reaction, the mixture was extracted with three times with ethyl acetate and washed with water. The crude material was purified by column chromatography using Heptanes/EA (90/10 to 80/20) solvent system. The solvent of the combined was removed under vacuum to afford 8-(7-chloroquinazolin-4-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (5.0 g, 92% yield) as a white solid.

Synthesis of 8-(7-isopropylquinazolin-4-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine

50 [0112]



[0113] 8-(7-chloroquinazolin-4-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (3.33 g, 9.25 mmol), 2'-(dicyclohexylphosphino)-N2,N2,N6,N6-tetramethyl-[1,1'-biphenyl]-2,6-diamine (CPhos) (0.32 g, 0.74 mmol) and diacetoxypalladium (0.08 g, 0.37 mmol) were diluted in dry THF (185 mL). The solution was cooled down to 0°C and a solution of isopropylzinc(II) bromide (28 mL, 13.9 mmol) was added dropwise. The reaction was stirred for 30 minutes at this temperature and then stirred overnight at room temperature. Upon completion, the reaction was quenched with a solution of ammonium

- stirred overnight at room temperature. Upon completion, the reaction was quenched with a solution of ammonium chloride, extracted with ethyl acetate and washed with Brine and water. The crude material was purified by column chromatography using Heptanes/EA/DCM (60/30/10 to 45/10/45) solvent system. The resulting solid still contained around 1% of *n*-propyl isomer. In order to remove that impurity, the product was purified by reverse phase column chromatography using Acetonitrile/Water (80/20). The removal of the n-propyl was successful but there was still some
- starting material left. The product was further purified two times by column chromatography using the same solvent system as described before. The title compound 8-(7-isopropylquinazolin-4-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine(1.6 g, 47% yield) was afforded as a white powder.

25 Synthesis of Ir(III) Dimer

[0114]

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[0115] 8-(7-isopropylquinazolin-4-yl)-2,6-dimethylbenzofuro[2,3-b]pyridine (1.6 g, 4.35 mmol) was solubilized in ethoxyethanol (13 mL) and Water (4 mL) and degassed by bubbling nitrogen gas for 30 minutes. Iridium chloride (0.38 g, 1.03 mmol) was then added to the solution and the reaction was refluxed under nitrogen for 24 hours. After cooling down to room temperature, the solid was filtered, washed with methanol and dried to give Ir(III) Dimer (1.0 g, 100 % yield) as an orange powder. There is still ligand left but will use without further purification.

Synthesis of Compound 56

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[0116]



In [0117] Ir(III) Dimer (1.0 g, 0.52 mmol) and 3,7-diethylnonane-4,6-dione (1.11 g, 5.21 mmol) were diluted in ethoxyethanol (20 mL) and the mixture was degassed by bubbling nitrogen gas. K₂CO₃ (0.72 g, 5.21 mmol) was then added and the reaction was stirred at room temperature overnight. The mixture was diluted with DCM, filtered through a pad of Celite, and washed with DCM. The crude material was purified by column chromatography (silica pre-treated with TEA) using Heptanes/DCM 90/10 solvent system. The product was triturated in methanol and the title compound was afforded as a red powder (0.16 g, 14 % yield).

Device Examples

[0118] The inventors have verified the benefits of the inventive compounds disclosed herein by fabricating experimental OLED devices. Device examples were made using Compound 24, Compound 56, and Compound 10 as an emitter material in the emissive layer. A Comparative Device was made using Comparative Compound 1 shown below:

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Comparative Compound 1

[0119] All example devices were fabricated by high vacuum (<10⁻⁷ Torr) thermal evaporation. The anode electrode is 1200 Å of indium tin oxide (ITO). The cathode consisted of 10 Å of LiF followed by 1,000 Å of Al. All devices are encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H₂O and O₂) immediately after fabrication, and a moisture getter was incorporated inside the package.

[0120] The organic stack of the device examples consisted of sequentially, from the ITO surface, 100 Å of LG101(purchased from LG chem) as the hole injection layer (HIL); 400 Å of 4,4'-bis[N-(1-naphthyl)-N-phenylamino]biphenyl (NPD) as the hole transporting layer (HTL); 300 Å of an emissive layer (EML) containing Compound H as a host (79%), a

- 50 stability dopant (SD) (18%), and Compound 24, Compound 56, or Compound 10 as an emitter; 100 Å of Compound H as a blocking layer; and 450 Å of Alq₃ (tris-8-hydroxyquinoline aluminum) as the ETL. The emitter was selected to provide the desired color and the stability dopant (SD) was mixed with the electron-transporting host and the emitter to help transport positive charge in the emissive layer. The Comparative Example was fabricated similarly to the device examples except that Comparative Compound 1 was used as the emitter in the EML. Table 2 shows the composition of the EML
- ⁵⁵ in the device, while the device results and data are summarized in Table 3. As used herein, NPD, compound H, SD, and Alq₃ have the following structures:



Table 2 Compounds of EML in the devices

15	Example	Host	Stability dopant	Emitter
10	Device Example 1			Compound 24
	Device Example 2		SD	Compound 56
	Device Example 3		30	Compound 10
20	Comparative example			Comparative compound 1

Table 3 Device results

	1931 CIE		λ max [nm]	FWHM [nm]	At 80mA/cm ² Relative LT _{95%} [h]
	х	У			
Device Example 1	0.63	0.37	606	42	3.1
Device Example 2	0.68	0.32	648	54	6.3
Device Example 3	0.60	0.39	614	88	8
Comparative example	0.64	0.36	612	52	1

- Table 3 summarizes the performance of the devices. The 1931 CIE values were measured at 10 mA/cm². The device operation lifetime measurements were performed at a constant dc current of 80 mA/cm² at room temperature with light output monitored as a function of time. The operational lifetimes defined at 95% of the initial luminance (LT_{95%}). The lifetime of the Comparative Example was set to 1 and the lifetimes of device examples are indicated as relative values compared to the Comparative Example (*i.e.*, a value of 2 indicates a LT_{95%} that is twice that of the Comparative Example).
- 40 Device Example 1 has a full width at half maximum (FWHM) that is 10 nm narrower than the Comparative Example. Device Example 1 also exhibited a LT^{95%} at 80mA/cm² more than three times longer than the Comparative Device. Device Example 2 exhibits a 42nm red shift of the peak wavelength compared to Device Example 1 and had a LT_{95%} at 80mA/cm² double that of Device Example 1. Device Example 3 exhibits a FWHM 36 nm wider than the Comparative Examiner, but also exhibits a LT_{95%} at 80mA/cm² that is 8 times the LT_{95%} of the Comparative Example.
- [0121] It is understood that the various embodiments described herein are by way of example only, and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore include variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.
 - [0122] The invention is further described by the following numbered paragraphs.

1. A compound having a formula $M(L_A)_x(L_B)_y(Lc)_z$: wherein ligand L_A is

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sulfonyl, phosphino, and combinations thereof; and wherein any adjacent substitutents of R^C, and R^D are optionally joined to form a fused ring.

- 2. The compound of paragraph 1, wherein M is selected from the group consisting of Ir, Rh, Re, Ru, Os, Pt, Au, and Cu.
 - 3. The compound of paragraph 1, wherein M is Ir.
 - 4. The compound of paragraph 1, wherein X is O.
- 5. The compound of paragraph 1, wherein the compound has the formula $M(L_A)_2(L_B)$.
 - 6. The compound of paragraph 1, wherein the compound has the formula $M(L_A)(L_C)_2$.

7. The compound of paragraph 1, wherein only one of A^1 to A^8 is N.

- 8. The compound of paragraph 1, wherein only one of A^5 to A^8 is N.
- 9. The compound of paragraph 1, wherein X^1 , X^2 , X^3 , and X^4 are C; and ring E is benzene.
- ²⁰ 10. The compound of paragraph 1, wherein (a) at least one of X¹, X², X³, and X⁴ is N, (b) ring E is heterocylic, or (c) both.
 - 11. The compound of paragraph 1, wherein L_A has the formula:



12. The compound of paragraph 1, wherein L_A has the formula:



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wherein R is selected from the group consisting of alkyl, cycloalkyl, and combinations thereof.

13. The compound of paragraph 12, wherein R is selected from the group consisting of methyl, ethyl, propyl, 1methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, cyclopentyl, cyclohexyl, partially or fully deuterated variants thereof,
and combinations thereof.

14. The compound of paragraph 1, wherein L_B has the formula:

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wherein R⁵, R⁶, R⁷, and R⁸ are independently selected from group consisting of alkyl, cycloalkyl, aryl, and heteroaryl; wherein at least one of R⁵, R⁶, R⁷, and R⁸ has at least two C atoms.

15. The compound of paragraph 1, wherein each R¹, R², R³, R^C, and R^D is independently selected from group consisting of hydrogen, deuterium, alkyl, cycloalkyl, and combinations thereof.

²⁰ 16. The compound of paragraph 1, wherein R³ is hydrogen.

17. The compound of paragraph 1, wherein each R¹, R², R³, R^C, and R^D is independently selected from the group consisting of methyl, ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, cyclobutyl, cyclopentyl, cyclobexyl, partially or fully deuterated variants thereof, and combinations thereof.

18. The compound of paragraph 1, wherein ring C is benzene, and ring D is pyridine.

19. The compound of paragraph 1, wherein the compound is selected from the group consisting of:



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and

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wherein each of R^F, R^G, R^H, R^I, R^J, and R^K are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfonyl, sulfonyl,



phosphino, and combinations thereof; and wherein $X^5,\,X^6,\,X^7$, and X^8 are C or N.

20. The compound of paragraph 1, wherein L_A is selected from the group consisting of L_{A1} to L_{A715} as described herein.



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22. The compound of paragraph 1, wherein L_B is selected from the group consisting of:



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23. The compound of paragraph 1, wherein the compound is selected from the group consisting of compounds 1 to 60 as described herein.

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24. A first device comprising a first organic light emitting device, the first organic light emitting device comprising:

an anode; a cathode; and an organic layer, disposed between the anode and the cathode, comprising a compound having a formula $M(L_A)_x(L_B)_y(L_C)_z$: wherein ligand L_A is

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sulfonyl, phosphino, and combinations thereof; and wherein any adjacent substitutents of R^C, and R^D are optionally joined to form a fused ring.

- 25. The first device of paragraph 24, wherein the first device is a consumer product.
 - 26. The first device of paragraph 24, wherein the first device is an organic light emitting device.
 - 27. The first device of paragraph 24, wherein the first device comprises a light panel.
- ¹⁰ 28. The first device of paragraph 24, wherein the organic layer is an emissive layer and the compound is an emissive dopant.

29. The first device of paragraph 24, wherein the organic layer is an emissive layer and the compound is a nonemissive dopant.

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30. The first device of paragraph 24, wherein the organic layer further comprises a host material.

31. The first device of paragraph 30, wherein the host material comprises a triphenylene containing benzo-fused thiophene or benzo-fused furan;

- ²⁰ wherein any substituent in the host material is an unfused substituent independently selected from the group consisting of C_nH_{2n+1} , OC_nH_{2n+1} , OAr_1 , $N(C_nH_{2n+1})_2$, $N(Ar_1)(Ar_2)$, $CH=CH-C_nH_{2n+1}$, $C=C-C_nH_{2n+1}$, Ar_1 , Ar_1-Ar_2 , $C_nH_{2n}-Ar_1$, or no substitution; wherein n is from 1 to 10; and
- wherein Ar₁ and Ar₂ are independently selected from the group consisting of benzene, biphenyl, naphthalene, triphenylene, carbazole, and heteroaromatic analogs thereof.

32. The first device of paragraph 30, wherein the host material comprises at least one chemical group selected from the group consisting of carbazole, dibenzothiphene, dibenzofuran, dibenzoselenophene, azacarbazole, aza-dibenzothiphene, aza-dibenzofuran, and azadibenzoselenophene.

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33. The first device of paragraph 30, wherein the host material is selected from the group consisting of:







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	wherein M is a metal having an atomic number greater than 40;
	wherein x is 1, or 2;
	wherein y is 0, 1, or 2;
15	wherein z is 0, 1, or 2;
	wherein x+y+z is the oxidation state of the metal M;
	wherein X ¹ , X ² , X ³ , X ⁴ , A ¹ , A ² , A ³ , A ⁴ , A ⁵ , A ⁶ , A ⁷ , and A ⁸ are C or N;
	wherein at least one of A ¹ , A ² , A ³ , A ⁴ , A ⁵ , A ⁶ , A ⁷ , and A ⁸ is N;
	wherein ring B is bonded to ring A through a C-C bond;
20	wherein M is bonded to ring A through a M-C bond;
	wherein X is O, S, or Se;
	wherein rings C, and D are each independently a 5 or 6-membered carbocyclic or heterocyclic ring;
	wherein R ^A represents mono, or di-substitution, or no substitution;
	wherein R ^B represents di, tri, or tetra-substitution;
25	wherein R ^C , R ^D , and R ⁴ each independently represent mono, di, tri, or tetra-substitution, or no substitution;
	wherein two adjacent R ^B form a six-member aromatic carbocyclic or heterocyclic ring E fused to ring B; wherein,
	when ring E is heterocyclic, the only heteroatom is nitrogen; wherein ring E can be further substituted by R ^E ; and
	wherein R ^E represents mono, di, tri, or tetra-substitution, or no substitution;

wherein each of R^A, R^B, R^C, R^D, R^E, R¹, R², R³, and R⁴ are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and

wherein any adjacent substitutents of R^C, and R^D are optionally joined to form a fused ring.

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Claims

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wherein ligand L_B is

^{1.} A compound having a formula $M(L_A)L_B)_y(L_C)_z :$ wherein ligand L_A is



R

wherein ligand L_C is



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- 8. The compound of any one of Claims 1 to 7, wherein X¹, X², X³, and X⁴ are C; and ring E is benzene.
- 9. The compound of any one of Claims 1 to 7, wherein (a) at least one of X¹, X², X³, and X⁴ is N, (b) ring E is heterocylic,

or (c) both.

10. The compound of any one of Claims 1 to 9, wherein L_{A} has the formula:



11. The compound of any one of Claims 1 to 10, wherein L_A has the formula:



12. The compound of any one of Claims 1 to 4 and 6 to 11, wherein L_B has the formula:



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wherein R⁵, R⁶, R⁷, and R⁸ are independently selected from group consisting of alkyl, cycloalkyl, aryl, and heteroaryl; wherein at least one of R⁵, R⁶, R⁷, and R⁸ has at least two C atoms.

- **13.** The compound of any one of Claims 1 to 3 and 5 to 11, wherein ring C is benzene, and ring D is pyridine.
- 14. The compound of any one of Claims 1 to 4 and 6 to 12, wherein the compound is selected from the group consisting of:





and

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wherein each of R^F, R^G, R^H, R^I, R^J, and R^K are independently selected from the group consisting of hydrogen, deuterium, halide, alkyl, cycloalkyl, heteroalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acids, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and wherein X⁵, X⁶, X⁷, and X⁸ are C or N.

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15. The compound of Claim 1, wherein L_A is selected from the group consisting of:

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wherein in L_{A1}, R = H, and R^A = H, in L_{A2}, R = H, and R^A = CH₃, in L_{A3}, R = H, and R^A = CD₃, in L_{A4}, R = CH₃, and R^A = H, in L_{A5}, R = CD₃, and R^A = H, in L_{A6}, R = CH₃, and R^A = CH₃, in L_{A7}, R = CD₃, and R^A = CD₃,

LA1 through LA13, each represented by the formula

In L_{A13}, R = isopropyi-*a*7, and R^{$$\circ$$} = CD₃,
L_{A27} through L_{A39}, each represented by the formula

 L_{A14} through L_{A26} , each represented by the formula

3-n



in L_{A15}, R = H, and R^A = CH₃, in L_{A16}, R = H, and R^A = CD₃, in L_{A17}, R = CH₃, and R^A = H, in L_{A17}, R = CD₃, and R^A = H, in L_{A19}, R = CD₃, and R^A = CH₃, in L_{A20}, R = CD₃, and R^A = CD₃, in L_{A21}, R = Ethyl, and R^A = CD₃, in L_{A22}, R = Ethyl, and R^A = CH₃, in L_{A23}, R = Ethyl-*d5*, and R^A = CD₃, in L_{A24}, R = isopropyl, and R^A = H, in L_{A25}, R = isopropyl, and R^A = CH₃, in L_{A26}, R = isopropyl-*d7*, and R^A = CD₃, L_{A40} through L_{A52}, each represented by the formula



	429 , 42 3,
	in $L_{A30:} R = CH_3$, and $R^A = H$,
15	in L_{A31} : R = CD ₃ , and R ^A = H,
	in L_{A32} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A33} : R = CD ₃ , and R ^A = CD ₃ ,
	in L _{A34} : R = Ethyl, and R ^A = H,
	in L_{A35} : R = Ethyl, and R ^A = CH ₃
20	in L_{A36} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
	in L _{A37} : R = isopropyl, and R ^A = H,
	in L_{A38} : R = isopropyl, and R ^A = CH ₃
	in L_{A39} : R = isopropyl-d7, and R ^A = CD ₃ ,

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 $_{25}$ L_{A53} through L_{A65}, each represented by the formula



	wherein in L_{A53} : R = H, and R ^A = H,
35	in L_{A54} : R = H, and R ^A = CH ₃ ,
	in L_{A55} : R = H, and R ^A = CD ₃ ,
	in L_{A56} : R = CH ₃ , and R ^A = H,
	in L_{A57} : R = CD ₃ , and R ^A = H,
40	in L_{A58} : R = CH ₃ , and R ^A = CH ₃
	in L_{AS9} : R = CD ₃ , and R ^A = CD ₃ ,
	in L _{A60} : R = Ethyl, and R ^A = H,
	in L_{A61} : R = Ethyl, and R^A = CH ₃ ,
	in L_{A62} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
45	in L_{A63} : R = isopropyl, and R ^A = H,
	in L_{A64} : R = isopropyl, and R ^A = CH ₃ ,
	in L_{A65} : R = isopropyl-d7, and R ^A = CD ₃ ,
	L_{A70} through L_{A01} , each represented by the formula



wherein in L_{A79}: R = H, and R^A = H, in L_{A80}: R = H, and R^A = CH_{3.}



wherein in L_{A40}: R = H, and R^A = H, in L_{A41}: R = H, and R^A = CH₃, in L_{A42}: R = H, and R^A = CD₃, in L_{A43}: R = CH₃, and R^A = H, in L_{A44}: R = CD₃, and R^A = H, in L_{A45}: R = CH₃, and R^A = CH₃, in L_{A46}: R = CD₃, and R^A = CD₃, in L_{A47}: R = Ethyl, and R^A = CH₃, in L_{A48}: R = Ethyl, and R^A = CH₃, in L_{A48}: R = Ethyl, and R^A = CH₃, in L_{A49}: R = Ethyl-*d5*, and R^A = CD₃, in L_{A50}: R = isopropyl, and R^A = H, in L_{A51}: R = isopropyl, and R^A = CH₃, in L_{A52}: R = isopropyl-*d7*, and R^A = CD₃, L_{A66} through L_{A78}, each represented by the formula







wherein in L_{A92} : R = H, and R^A = H, in L_{A93} : R = H, and = CH₃.

(continued)

	in L _{A81} : R = H, and R ^A = CD _{3,}
	in L_{A82} : R = CH ₃ , and R ^A = H,
5	in L_{A83} : R = CD ₃ , and R ^A = H,
	in L_{A84} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A85} : R = CD ₃ , and R ^A = CD ₃ ,
	in L_{A86} : R = Ethyl, and R ^A = H,
	in L_{A87} : R = Ethyl, and R ^A = CH ₃
0	in L_{A88} : R = Ethyl-d5, and R ^A = CD ₃ ,
	in L_{A89} : R = isopropyl, and R ^A = H,
	in L_{A90} : R = isopropyl, and R ^A = CH _{3.}
	in L_{A91} : R = isopropyl-d7, and R ^A = CD ₃ ,

 $_{15}$ L_{A105} through L_{A117}, each represented by the formula



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	wherein in L _{A105} : R = H, and R ^A = H,
	in L_{A106} : R = H, and R ^A = CH ₃ ,
25	in L_{A107} : R = H, and R ^A = CD ₃ ,
	in L_{A108} : R = CH ₃ , and R ^A = H,
	in L_{A109} : R = CD ₃ , and R ^A = H,
	in L_{A110} : R = CH ₃ , and R ^A = CH ₃ ,
30	in L_{A111} : R = CD ₃ , and R ^A = CD ₃ ,
	in L _{A112} : R = Ethyl, and R ^A = H,
	in L_{A113} : R = Ethyl, and R ^A = CH ₃ ,
	in $L_{A11}4$: R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
	in $L_{A11}5$: R = isopropyl, and R ^A = H,
35	in L_{A116} : R = isopropyl, and R ^A = CH ₃ ,
	in L_{A117} : R = isopropyl-d7, and R ^A = CD ₃

 L_{A131} through $L_{A143},$ each represented by the formula

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	wherein in L_{A131} : R = H, and R ^A = H,
	in L_{A132} : R = H, and R ^A = CH ₃ ,
	in L_{A133} : R = H, and R ^A = CD ₃ ,
50	in L_{A134} : R = CH ₃ , and R ^A = H,
00	in L_{A135} : R = CD ₃ , and R ^A = H,
	in L_{A136} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A137} : R = CD ₃ , and R ^A = CD ₃ ,
	in L_{A138} : R = Ethyl, and R ^A = H,
55	in L_{A139} : R = Ethyl, and R ^A = CH ₃
	in L_{A140} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
	in L_{A141} : R = isopropyl, and R ^A = H,

in L_{A94} : R = H, and R^A = CD₃, in L_{A95} : R = CH₃, and R^A = H, in L_{A96} : R = CD₃, and R^A = H, in L_{A97} : R = CH₃, and R^A = CH₃, in L_{A98} : R = CD₃, and R^A = CD₃, in L_{A98} : R = Ethyl, and R^A = H, in L_{A100} : R = Ethyl, and R^A = CH₃, in L_{A101} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A102} : R = isopropyl, and R^A = H, in L_{A103} : R = isopropyl, and R^A = CH₃, in L_{A104} : R = isopropyl-*d7*, and R^A = CD₃,



wherein in L_{A118} : R = H, and R^A = H, in L_{A119} : R = H, and R^A = CH₃, in L_{A120} : R = H, and R^A = CD₃, in L_{A121} : R = CH₃, and R^A = H, in L_{A122} : R = CD₃, and R^A = H, in L_{A123} : R = CH₃, and R^A = CH₃, in L_{A124} : R = CD₃, and R^A = CD₃, in L_{A125} : R = Ethyl, and R^A = H, in L_{A126} : R = Ethyl, and R^A = CH₃, in L_{A127} : R = Ethyl, and R^A = CH₃, in L_{A127} : R = Ethyl, and R^A = CH₃, in L_{A128} : R = isopropyl, and R^A = CD₃, in L_{A129} : R = isopropyl, and R^A = CH₃, in L_{A129} : R = isopropyl-*d*7, and R^A = CD₃, L_{A144} through L_{A156} , each represented by the formula



wherein in L_{A144} : R = H, and R^A = H, in L_{A145} : R = H, and R^A = CH₃, in L_{A146} : R = H, and R^A = CD₃, in L_{A147} : R = CH₃, and R^A = H, in L_{A148} : R = CD₃, and R^A = H, in L_{A149} : R = CH₃, and R^A = CH₃, in L_{A150} : R = CD₃, and R^A = CD₃, in L_{A151} : R = Ethyl, and R^A = H, in L_{A152} : R = Ethyl, and R^A = CH₃, in L_{A152} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A154} : R = isopropyl, and R^A = H, (continued)

in L_{A142}: R = isopropyl, and R^A = CH₃, in L_{A143}: R = isopropyl-*d*7, and R^A = CD₃, L_{A157} through L_{A169}, each represented by the formula

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$$N$$
 R R^A

	wherein in L _{A157} : R = H, and R ^A = H,
15	in L_{A158} : R = H, and R ^A = CH ₃
	in L_{A159} : R = H, and R ^A = CD ₃ ,
	in L_{A160} : R = CH ₃ , and R ^A = H,
	in L_{q161} : R = CD ₃ , and R ^A = H,
20	in L_{A162} : R = CH ₃ , and R ^A = CH ₃ ,
20	in L_{A163} : R = CD ₃ , and R ^A = CD ₃ ,
	in L_{A164} : R = Ethyl, and R ^A = H,
	in L_{A165} : R = Ethyl, and R ^A = CH ₃
	in L_{A166} ; R = Ethyl- <i>d5</i> , and R ^A = CD ₃ .
25	in L_{A167} : R = isopropyl, and R ^A = H,
	in L_{A168} : R = isopropyl, and R ^A = CH ₃
	in L_{A169} : R = isopropyl-d7, and R ^A = CD ₃ ,
	L_{A183} through L_{A195} , each represented by the formula



wherein in L_{A170} : R = H, and R^A = H, in L_{A171} : R = H, and R^A = CH₃, in L_{A172} : R = H, and R^A = CD₃, in L_{A173} : R = CH₃, and R^A = H, in L_{A174} : R = CD₃, and R^A = H, in L_{A175} : R = CH₃, and R^A = CH₃, in L_{A176} : R = CD₃, and R^A = CD₃, in L_{A177} : R = Ethyl, and R^A = H, in L_{A177} : R = Ethyl, and R^A = CH₃, in L_{A177} : R = Ethyl, and R^A = CH₃, in L_{A179} : R = Ethyl, and R^A = CH₃, in L_{A179} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A180} : R = isopropyl, and R^A = H, in L_{A181} : R = isopropyl, and R^A = CH₃, in L_{A182} : R = isopropyl-*d7*, and R^A = CD₃, L_{A196} through L_{A208} , each represented by the formula



herein in L_{A196} : R = H, and R ^A = H,
in L_{A197} : R = H, and R ^A = CH ₃ .
in L_{A198} : R = H, and R ^A = CD ₃
in L_{A199} : R = CH ₃ , and R ^A = H,
in L_{A200} : R = CD ₃ , and R ^A = H,
in L_{A201} : R = CH ₃ , and R ^A = CH ₃ ,
in L_{A202} : R = CD ₃ , and R ^A = CD ₃ ,
in L_{A203} : R = Ethyl, and R ^A = H,
in L_{A204} : R = Ethyl, and R ^A = CH ₃ ,
in L_{A205} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
in L_{A206} : R = isopropyl, and R ^A = H,
in L_{A207} : R = isopropyl, and R ^A = CH ₃ ,
in L_{A208} : R = isopropyl-d7, and R ^A = CD ₃ ,
L_{A222} through $L_{A234},$ each represented by the formula

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	$R \rightarrow R^{\wedge}$
	wherein in L_{A183} : R = H, and R ^A = H,
	in L_{A84} : R = H, and R ^A = CH ₃ ,
40	in L_{A185} : R = H, and R ^A = CD ₃ ,
	in L_{A186} : R = CH ₃ , and R ^A = H,
	in L_{A187} : R = CD ₃ , and R ^A = H,
	in L_{A188} : R = CH ₃ , and R ^A = CH ₃ ,
45	in L_{A189} : R = CD ₃ , and R ^A = CD ₃ ,
	in L_{A190} : R = Ethyl, and R ^A = H,
	in L_{A191} : R = Ethyl, and R ^A = CH ₃ ,
	in L_{A192} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
	in L_{A193} : R = isopropyl, and R ^A = H,
50	in L_{A194} : R = isopropyl, and R ^A = CH ₃ ,
	in L_{A195} : R = isopropyl-d7, and R ^A = CD ₃ ,
	$\rm L_{A209}$ through $\rm L_{A221},$ each represented by the formula





wherein in L_{A222} : R = H, and R^A = H, in L_{A223} : R = H, and R^A = CH₃, in L_{A224} : R = H, and R^A = CD₃, in L_{A225} : R = CH₃, and R^A = H, in L_{A226} : R = CD₃, and R^A = H, in L_{A227} : R = CH₃, and R^A = CH₃, in L_{A228} : R = CD₃, and R^A = CD₃, in L_{A229} : R = Ethyl, and R^A = CH₃, in L_{A230} : R = Ethyl, and R^A = CH₃, in L_{A231} : R = Ethyl, and R^A = CH₃, in L_{A231} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A232} : R = isopropyl, and R^A = H, in L_{A233} : R = isopropyl, and R^A = CH₃, in L_{A234} : R = isopropyl-*d7*, and R^A = CD₃, L_{A248} through L_{A260} , each represented by the formula



wherein in L_{A248} : R = H, and R ^A = H,
in L_{A249} : R = H, and R ^A = CH ₃ ,
in L_{A250} : R = H, and R ^A = CD ₃ ,
in L_{A251} : R = CH ₃ , and R ^A = H,
in L_{A252} : R = CD ₃ , and R ^A = H,
in L_{A253} : R = CH ₃ , and R ^A = CH ₃ ,
in L_{A254} : R = CD ₃ , and R ^A = CD ₃ ,
in L _{A255} : R = Ethyl, and R ^A = H,
in L_{A256} : R = Ethyl, and R ^A = CH ₃ ,
in L_{A257} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
in L _{A258} : R = isopropyl, and R ^A = H,
in L_{A259} : R = isopropyl, and R ^A = CH ₃ ,
in L_{A260} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ ,
L_{A274} through $L_{A286},$ each represented by the formula





wherein in L_{A274} : R = H, and R^A = H, in L_{A275} : R = H, and R^A = CH₃, in L_{A276} : R = H, and R^A = CD₃, in L_{A277} : R = CH₃, and R^A = H, in L_{A278} : R = CD₃, and R^A = H, in L_{A279} : R = CH₃, and R^A = CH₃, in L_{A280} : R = CD₃, and R^A = CD₃, in L_{A281} : R = Ethyl, and R^A = H, in L_{A282} : R = Ethyl, and R^A = CH₃. in L_{A282} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A284} : R = isopropyl, and R^A = H, in L_{A285} : R = isopropyl, and R^A = CH₃, in L_{A285} : R = isopropyl-*d7*, and R^A = CD₃, L_{A300} through L_{A312} , each represented by the formula







wherein in L_{A326} : R = H, and R^A = H, in L_{A327} : R = H, and R^A = CH₃, in L_{A328} : R = H, and R^A = CD₃, in L_{A329} : R = CH₃, and R^A = H, in L_{A330} : R = CD₃, and R^A = H, in L_{A331} : R = CH₃, and R^A = CH₃, in L_{A332} : R = CD₃, and R^A = CD₃, in L_{A332} : R = Ethyl, and R^A = H, in L_{A334} : R = Ethyl, and R^A = CH₃, in L_{A335} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A336} : R = isopropyl, and R^A = H, in L_{A337} : R = isopropyl, and R^A = CH₃, in L_{A337} : R = isopropyl, and R^A = CH₃, in L_{A338} : R = isopropyl-*d7*, and R^A = CD₃,

 L_{A339} through $L_{A351},$ each represented by the formula



40	in L_{A340} : R = H, and R ^A = CH ₃ ,
	in L_{A341} : R = H, and R ^A = CD ₃ ,
	in L_{A342} : R = CH ₃ , and R ^A = H,
	in L_{A343} R = CD ₃ , and R ^A = H,
	in L_{A344} : R = CH ₃ , and R ^A = CH ₃ ,
	in L_{A345} : R = CD ₃ , and R ^A = CD ₃ ,
45	in L_{A346} : R = Ethyl, and R ^A = H,
	in L_{A347} : R = Ethyl, and R ^A = CH ₃ ,
50	in L_{A348} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
	in L_{A349} : R = isopropyl, and R ^A = H,
	in L_{A350} : R = isopropyl, and R ^A = CH ₃ ,
	in L_{A351} : R = isopropyl-d7, and R ^A = CD ₃ ,
	L_{A365} through L_{A377} , each represented by the formula

 L_{A352} through $L_{A364},$ each represented by the formula



wherein in L_{A352} : R = H, and R^A = H, in L_{A353} : R = H, and R^A = CH₃, in L_{A354} : R = H, and R^A = CD₃, in L_{A355} : R = CH₃, and R^A = H, in L_{A356} : R = CD₃, and R^A = H, in L_{A357} : R = CH₃, and R^A = CH₃, in L_{A358} : R = CD₃, and R^A = CD₃, in L_{A359} : R = Ethyl, and R^A = H, in L_{A360} : R = Ethyl, and R^A = CH₃, in L_{A361} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A362} : R = isopropyl, and R^A = H, in L_{A363} : R = isopropyl, and R^A = CH₃, in L_{A364} : R = isopropyl-*d7*, and R^A = CD₃, L_{A378} through L_{A390} , each represented by the formula





wherein in L_{A378} : R = H, and R^A = H, in L_{A379} : R = H, and R^A = CH₃, in L_{A380} : R = H, and R^A = CD₃, in L_{A381} : R = CH₃, and R^A = H, in L_{A382} : R = CD₃, and R^A = H, in L_{A383} : R = CH₃, and R^A = CH₃, in L_{A384} : R = CD₃, and R^A = CD₃, in L_{A385} : R = Ethyl, and R^A = H, in L_{A386} : R = Ethyl, and R^A = CH₃, in L_{A387} : R = Ethyl, and R^A = CH₃, in L_{A387} : R = Ethyl, and R^A = CH₃, in L_{A388} : R = isopropyl, and R^A = CD₃, in L_{A388} : R = isopropyl, and R^A = CH₃, in L_{A389} : R = isopropyl-*d7*, and R^A = CD₃, L_{A404} through L_{A416} , each represented by the formula



wherein in L_{A404} : R = H, and R^A = H, in L_{A405} : R = H, and R^A = CH₃, in L_{A406} : R = H, and R^A = CD₃, in L_{A407} : R = CH₃, and R^A = H, in L_{A408} : R = CD₃, and R^A = H, in L_{A408} : R = CD₃, and R^A = CH₃, in L_{A410} : R = CD₃, and R^A = CD₃, in L_{A411} : R = Ethyl, and R^A = H, in L_{A412} : R = Ethyl, and R^A = CH₃, in L_{A413} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A415} : R = isopropyl, and R^A = H, in L_{A415} : R = isopropyl, and R^A = CH₃, in L_{A416} : R = isopropyl-*d7*, and R^A = CD₃, L_{A430} through L_{A442} , each represented by the formula



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15	wherein in L_{A469} : R = H, and R ^A = H, in L_{A470} : R = H, and R ^A = CH ₃ , in L_{A471} : R = H, and R ^A = CD ₃ , in L_{A472} : R = CH ₃ , and R ^A = H, in L_{A472} : R = CD ₂ , and R ^A = H.
20	in L _{A473} : R = CH ₃ , and R ^A = CH ₃ , in L _{A475} : R = CD ₃ , and R ^A = CD ₃ , in L _{A476} : R = Ethyl, and R ^A = H, in L _{A477} : R = Ethyl, and R ^A = CH ₃ ,
25	In L _{A478} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ , in L _{A479} : R = isopropyl, and R ^A = H, in L _{A480} : R = isopropyl, and R ^A = CH ₃ , in L _{A481} : R = isopropyl- <i>d</i> 7, and R ^A = CD ₃ , L _{A495} through L _{A507} , each represented by the formula
30	
35	$R \rightarrow R^A$ wherein in L _{Ador} : $R = H$, and $R^A = H$.
40	in L_{A496} : R = H, and R ^A = CH ₃ , in L_{A497} : R = H, and R ^A = CD ₃ , in L_{A498} : R = CH ₃ , and R ^A = H, in L_{A499} : R = CD ₃ , and R ^A = H, in L_{A499} : R = CH ₂ , and R ^A = CH ₂ ,
45	in L _{A501} : R = CD ₃ , and R ^A = CD ₃ , in L _{A501} : R = Ethyl, and R ^A = H, in L _{A503} : R = Ethyl, and R ^A = CH ₃ , in L _{A504} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
50	in L_{A505} : $R =$ isopropyl, and $R^{A} = H$, in L_{A506} : $R =$ isopropyl, and $R^{A} = CH_{3}$, in L_{A507} : $R =$ isopropyl- <i>d7</i> , and $R^{A} = CD_{3}$, L_{A521} through L_{A533} , each represented by the formula



wherein in L_{A482} : R = H, and R^A = H, in L_{A483} : R = H, and R^A = CH₃, in L_{A484} : R = H, and R^A = CD₃, in L_{A485} : R = CH₃, and R^A = H, in L_{A486} : R = CD₃, and R^A = H, in L_{A486} : R = CD₃, and R^A = CH₃, in L_{A487} R = CH₃, and R^A = CD₃, in L_{A489} : R = Ethyl, and R^A = H, in L_{A490} : R = Ethyl, and R^A = CH₃, in L_{A491} : R = Ethyl-*d5*, and R^A = CD₃, in L_{A492} : R = isopropyl, and R^A = H, in L_{A493} : R = isopropyl, and R^A = CH₃, in L_{A493} : R = isopropyl-*d7*, and R^A = CD₃, L_{A508} through L_{A520} , each represented by the formula







 L_{A573} through L_{A585} , each represented by the formula

 L_{A586} through L_{A598} , each represented by the formula

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15	wherein in L_{A573} : R = H, and R ^A = H, in L_{A574} : R = H, and R ^A = CH ₃ , in L_{A575} : R = H, and R ^A = CD ₃ , in L_{A576} : R = CH ₃ , and R ^A = H, in L_{A577} : R = CD ₃ , and R ^A = H,	v ii ii ii
20	in L_{A578} : R = CH ₃ , and R ^A = CH ₃ , in L_{A579} : R = CD ₃ , and R ^A = CD ₃ , in L_{A580} : R = Ethyl, and R ^A = H, in L_{A581} : R = Ethyl, and R ^A = CH ₃ , in L_{A581} : R = Ethyl- <i>d5</i> and R ^A = CD ₃	iı iı iı iı
25	in L_{A582} : R = isopropyl, and R ^A = H, in L_{A584} : R = isopropyl, and R ^A = CH ₃ , in L_{A585} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ , L_{A599} through L_{A611} , each represented by the formula	iı iı iı L
30		
35	$R \rightarrow R^{A}$	
40	in L_{A600} : R = H, and R ^A = CH ₃ , in L_{A601} : R = H, and R ^A = CD ₃ , in L_{A602} : R = CH ₃ , and R ^A = H,	v ii ii ii
	in L_{A603} : R = CD ₃ , and R ^A = H, in L_{A604} : R = CH ₃ , and R ^A = CH ₃ , in L_{A605} : R = CD ₃ , and R ^A = CD ₃ , in L_{A606} : R = Ethyl, and R ^A = H,	ii ii ii ii
45	in L_{A607} : R = Etnyl, and R ^A = CH ₃ , in L_{A608} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ , in L_{A609} : R = isopropyl, and R ^A = H, in L_{A610} : R = isopropyl, and R ^A = CH ₃ ,	ii ii ii
50	in L_{A611} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ , L_{A625} through L_{A637} , each represented by the formula	iı L



wherein in L_{A586} : R = H, and R ^A = H,
n L _{A587} : R = H, and R ^A = CH ₃ ,
n L _{A588} : R = H, and R ^A = CD ₃ ,
n L_{A589} : R = CH ₃ , and R ^A = H,
n L_{A590} : R = CD ₃ , and R ^A = H,
n L_{A591} : R = CH ₃ , and R ^A = CH ₃ ,
n L_{A592} : R = CD ₃ , and R ^A = CD ₃ ,
n L _{A593} : R = Ethyl, and R ^A = H,
n L _{A594} : R = Ethyl, and R ^A = CH ₃ ,
n L _{A595} : R = Ethyl- $d5$, and R ^A = CD ₃ ,
n L _{A596} : R = isopropyl, and R ^A = H,
n L_{A597} : R = isopropyl, and R ^A = CH ₃ ,
n L _{A598} : R = isopropyl- <i>d7</i> , and R ^A = CD3,
$_{-A612}$ through L _{A624} , each represented by the formula





	(continued)			
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10		R-C-RA		
15	wherein in L_{A625} : R = H, and R ^A = H, in L_{A626} : R = H, and R ^A = CH ₃ , in L_{A627} : R = H, and R ^A = CD ₃ , in L_{A628} : R = CH ₃ , and R ^A = H, in L_{A629} : R = CD ₃ , and R ^A = H, in L_{A630} : R = CH ₃ , and R ^A = CH ₃ ,	wherein in L_{A638} : R = H, and R ^A = H, in L_{A639} : R = H, and R ^A = CH ₃ , in L_{A640} : R = H, and R ^A = CD ₃ , in L_{A641} : R = CH ₃ , and R ^A = H, in L_{A642} : R = CD ₃ , and R ^A = H, in L_{A643} : R = CH ₃ , and R ^A = CH ₃ ,		
20	in L_{A631} : R = CD ₃ , and R ^A = CD ₃ , in L_{A632} : R = Ethyl, and R ^A = H, in L_{A633} : R = Ethyl, and R ^A = CH ₃ , in L_{A634} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,	in L_{A644} : R = CD ₃ , and R ^A = CD ₃ , in L_{A645} : R = Ethyl, and R ^A = H, in L_{A646} : R = Ethyl, and R ^A = CH ₃ , in L_{A647} : R Ethyl- <i>d5</i> , and R ^A CD ₃ ,		
25	in L_{A635} : R = isopropyl, and R ^A = H, in L_{A636} : R = isopropyl, and R ^A = CH ₃ , in L_{A637} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ , L_{A651} through L_{A663} , each represented by the formula	in L_{A648} : R = isopropyl, and R ^A = H, in L_{A649} : R = isopropyl, and R ^A = CH ₃ , in L_{A650} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ , L_{A664} through L_{A676} , each represented by the formula		
30 35				
40	wherein in L_{A651} : R = H, and R ^A = H, in L_{A652} : R = H, and R ^A = CH ₃ , in L_{A653} : R = H, and R ^A = CD ₃ , in L_{A654} : R = CH ₂ , and R ^A = H.	wherein in L_{A664} : R = H, and R ^A = H, in L_{A665} : R = H, and R ^A = CH ₃ , in L_{A666} : R = H, and R ^A = CD ₃ , in L_{A667} : R = CH ₂ , and R ^A = H.		
	in L_{A656} : R = CD ₃ , and R ^A = H, in L_{A656} : R = CH ₃ , and R ^A = CH ₃ , in L_{A657} : R = CD ₃ , and R ^A = CD ₃ , in L_{A658} : R = Ethyl, and R ^A = H,	in L_{A668} : R = CD ₃ , and R ^A = H, in L_{A669} : R = CH ₃ , and R ^A = CH ₃ , in L_{A670} : R = CD ₃ , and R ^A = CD ₃ , in L_{A671} : R = Ethyl, and R ^A = H.		
45	in L _{A660} : R = Ethyl, and R ^A = CH ₃ , in L _{A660} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ , in L _{A661} : R = isopropyl, and R ^A = H, in L _{A662} : R = isopropyl, and R ^A = CH ₃ ,	in L_{A672} : R = Ethyl, and R ^A = CH ₃ , in L_{A673} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ , in L_{A674} : R = isopropyl, and R ^A = H, in L_{A675} : R = isopropyl, and R ^A = CH ₃ ,		
50	in L_{A663} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ , L_{A677} through L_{A689} , each represented by the formula	in L_{A676} : R = isopropyl- <i>d7</i> , and R ^A = $CD_{3,}$ L_{A690} through L_{A702} , each represented by the formula		

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10	
15	wherein in L_{A677} : R = H, and R ^A = H, in L_{A678} : R = H, and R ^A = CH ₃ , in L_{A679} : R = H, and R ^A = CD ₃ , in L_{A680} : R = CH ₃ , and R ^A = H, in L_{A681} : R = CD ₃ , and R ^A = H,
20	in L_{A682} : R = CH ₃ , and R ^A = CH ₃ , in L_{A683} : R = CD ₃ , and R ^A = CD ₃ , in L_{A684} : R = Ethyl, and R ^A = H, in L_{A685} : R = Ethyl, and R ^A = CH ₃ , in L_{A686} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
25	in L_{A687} : R = isopropyl, and R ^A = H, in L_{A688} : R = isopropyl, and R ^A = CH ₃ , in L_{A689} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ , L_{A703} through L_{A715} , each represented by the formula
30	
25	
30	wherein in L _{A703} : R = H, and R ^A = H, in L _{A704} : R = H, and R ^A = CH ₃ , in L _{A705} : R = H, and R ^A = CD ₃ ,
40	in L_{A706} : R = CH ₃ , and R ^A = H, in L_{A707} : R = CD ₃ , and R ^A = H, in L_{A708} : R = CH ₃ , and R ^A = CH ₃ , in L_{A709} : R = CD ₃ , and R ^A = CD ₃ ,
45	in L_{A710} : R = Ethyl, and R ^A = H, in L_{A711} : R = Ethyl, and R ^A = CH ₃ , in L_{A712} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ , in L_{A713} : R = isopropyl, and R ^A = H, in L_{A714} : R = isopropyl, and R ^A = CH ₃ ,
50	in L_{A715} : R = isopropyl- <i>d7</i> , and R ^A = CD ₃ ,



wherein in L_{A690} : R = H, and R ^A = H,
in L_{A691} : R = H, and R ^A = CH ₃ ,
in L_{A692} : R = H, and R ^A = CD ₃ ,
in L_{A693} : R = CH ₃ , and R ^A = H,
in L_{A694} : R = CD ₃ , and R ^A = H,
in L_{A695} : R = CH ₃ , and R ^A = CH ₃ ,
in L_{A696} : R = CD ₃ , and R ^A = CD ₃ ,
in L _{A697} : R = Ethyl, and R ^A = H,
in L_{A698} : R = Ethyl, and R ^A = CH ₃ ,
in L_{A699} : R = Ethyl- <i>d5</i> , and R ^A = CD ₃ ,
in L_{A700} : R = isopropyl, and R ^A = H,
in L_{A701} : R = isopropyl, and R ^A = CH ₃ ,
in L _{A702} : R = isopropyl- <i>d</i> 7, and R ^A = CD ₃ , and

16. The compound of Claim 1 or 15, wherein ${\rm L}_{\rm C}$ is selected from the group consisting of:







18. The compound of Claim 1, wherein the compound is selected from the group consisting of:













- 45 **19.** A first device comprising a first organic light emitting device, the first organic light emitting device comprising:
 - an anode; a cathode; and an organic layer, disposed between the anode and the cathode, comprising a compound as defined in any one of claims 1 to 18.

20. A formulation comprising a compound as defined in any one of claims 1 to 19.





FIGURE 1



FIGURE 2







Ligand L_A

Ligand L_B

Ligand $L_{\rm C}$





EUROPEAN SEARCH REPORT

Application Number

EP 15 16 5591

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